10/767784
=> file registry
FILE 'REGISTRY' ENTERED AT 13:51:39 ON 02 MAY 2007
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STRUCTURE FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8
DICTIONARY FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

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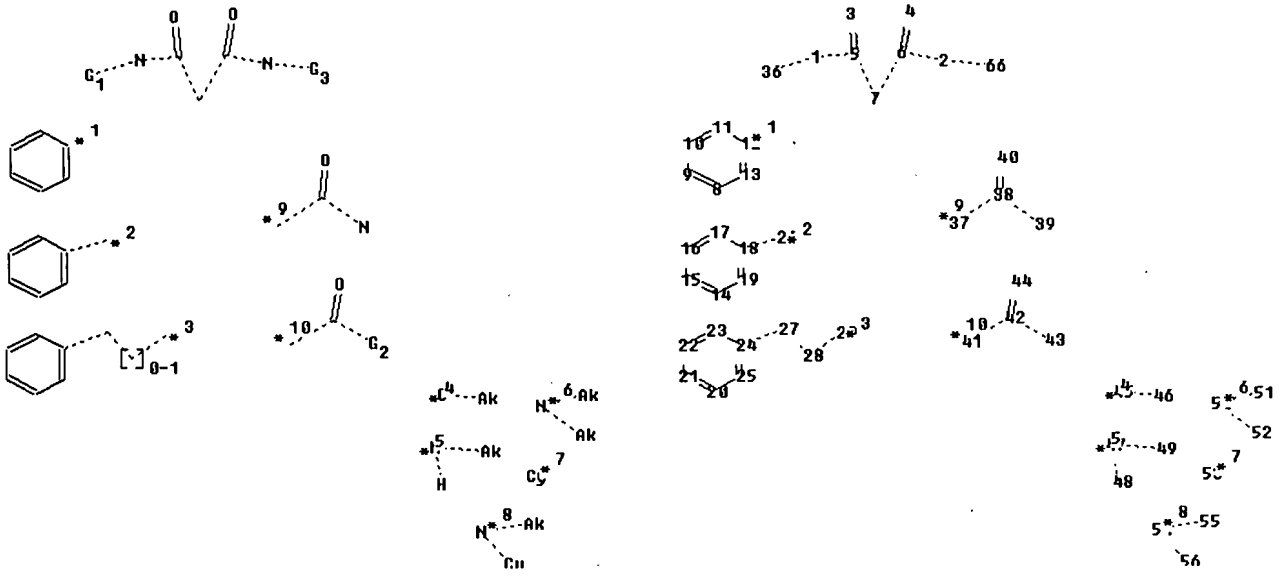
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

Uploading L1.str



chain nodes :
1 2 3 4 5 6 7 36 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 66
ring nodes :
8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 37 38 39

ring/chain nodes :

```
26  27  28  29
chain bonds :
1-5  1-36  2-6  2-66  3-5  4-6  5-7  6-7  18-26  24-27  38-40  41-42  42-43  42-44
45-46  47-48  47-49  50-51  50-52  54-55  54-56
ring/chain bonds :
27-28  28-29
ring bonds :
8-9  8-13  9-10  10-11  11-12  12-13  14-15  14-19  15-16  16-17  17-18  18-19  20-
21
20-25  21-22  22-23  23-24  24-25  37-38  38-39
exact/norm bonds :
1-5  1-36  2-6  2-66  3-5  4-6  5-7  6-7  18-26  24-27  27-28  28-29  37-38  38-39
38-40  41-42  42-43  42-44  45-46  47-48  47-49  50-51  50-52  54-55  54-56
normalized bonds :
8-9  8-13  9-10  10-11  11-12  12-13  14-15  14-19  15-16  16-17  17-18  18-19  20-
21
20-25  21-22  22-23  23-24  24-25


G1:[*1],[*2],[*3]

G2:[*4],[*5],[*6],[*7],[*8]

G3:[*9],[*10]

Match level :
1:CLASS  2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS  8:Atom  9:Atom
10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom
20:Atom  21:Atom
22:Atom  23:Atom  24:Atom  25:Atom  26:CLASS  27:CLASS  28:CLASS  29:CLASS
36:CLASS  37:Atom
38:Atom  39:Atom  40:CLASS  41:CLASS  42:CLASS  43:CLASS  44:CLASS  45:CLASS
46:CLASS  47:CLASS
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56:Atom  66:CLASS



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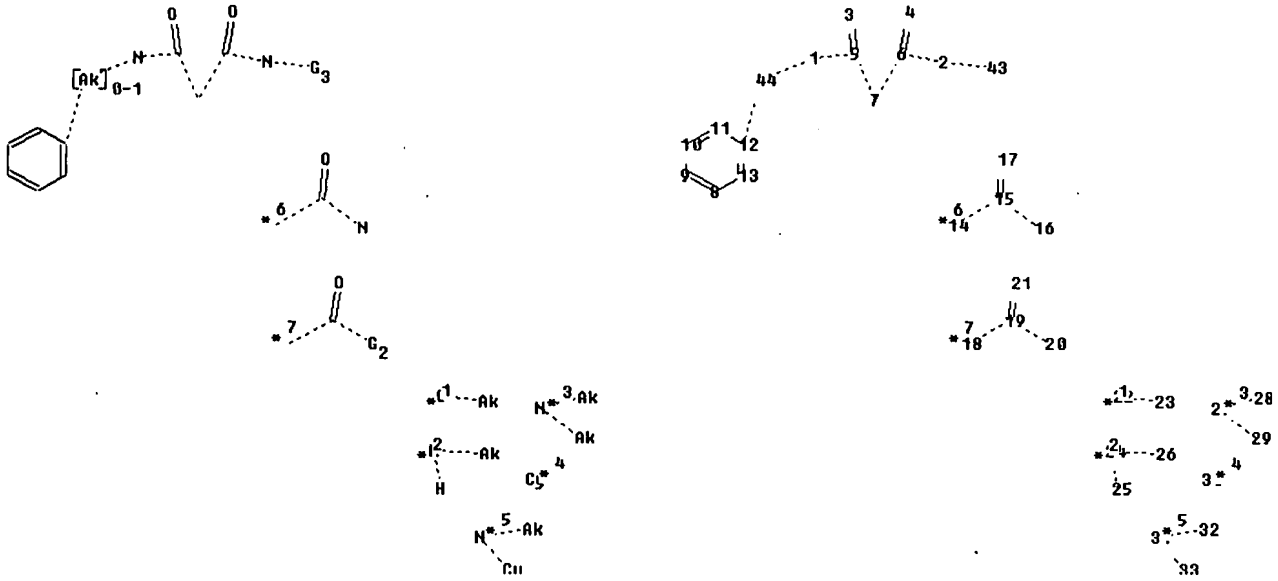


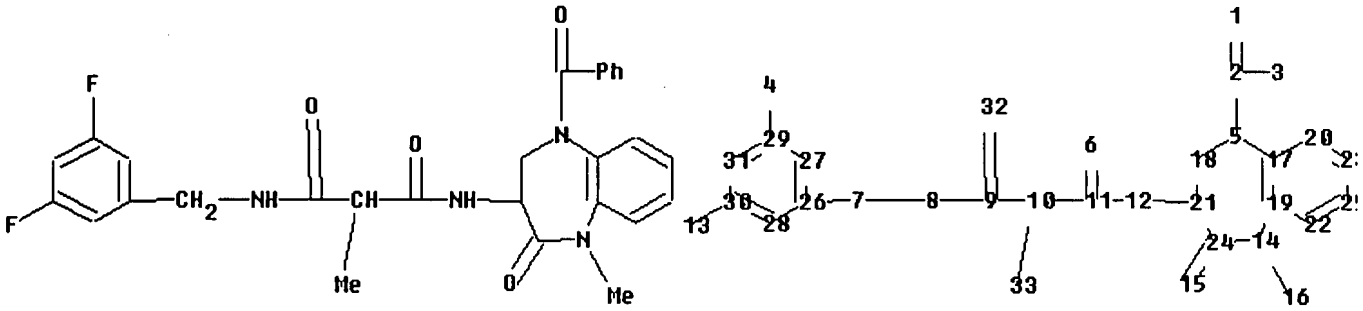
chain nodes :
1 2 3 4 5 6 7 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31
32 33 43 44
ring nodes :
8 9 10 11 12 13 14 15 16
chain bonds :
1-5 1-44 2-6 2-43 3-5 4-6 5-7 6-7 12-44 15-17 18-19 19-20 19-21 22-23
24-25 24-26 27-28 27-29 31-32 31-33
ring bonds :
8-9 8-13 9-10 10-11 11-12 12-13 14-15 15-16
exact/norm bonds :
1-5 1-44 2-6 2-43 3-5 4-6 5-7 6-7 12-44 14-15 15-16 15-17 18-19 19-20
19-21 22-23 24-25 24-26 27-28 27-29 31-32 31-33
normalized bonds :
8-9 8-13 9-10 10-11 11-12 12-13
isolated ring systems :
containing 8 :

G2:[*1],[*2],[*3],[*4],[*5]

G3:[*6],[*7]

Connectivity :
44:2 E exact RC ring/chain
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom
10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS
20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:CLASS 30:Atom
31:CLASS 32:CLASS 33:Atom 43:CLASS 44:CLASS

Uploading L34.str

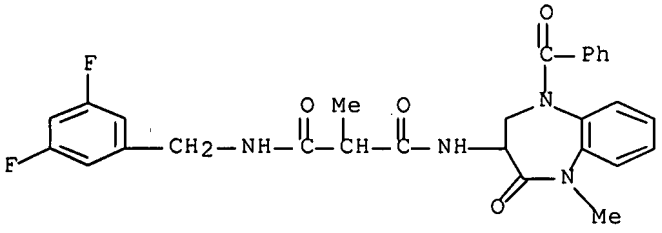


chain nodes :
1 2 3 4 6 7 8 9 10 11 12 13 15 16 32 33
ring nodes :
5 14 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31
chain bonds :
1-2 2-5 2-3 4-29 6-11 7-8 7-26 8-9 9-10 9-32 10-11 10-33 11-12 12-21
13-30 14-16 15-24
ring bonds :
5-17 5-18 14-19 14-24 17-19 17-20 18-21 19-22 20-23 21-24 22-25 23-25
26-27 26-28 27-29 28-30 29-31 30-31
exact/norm bonds :
1-2 2-5 5-17 5-18 6-11 8-9 9-32 11-12 12-21 14-19 14-24 15-24 18-21
21-24
exact bonds :
2-3 4-29 7-8 7-26 9-10 10-11 10-33 13-30 14-16
normalized bonds :
17-19 17-20 19-22 20-23 22-25 23-25 26-27 26-28 27-29 28-30 29-31 30-31

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:Atom 15:CLASS 16:CLASS 17:Atom 18:Atom
19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom
30:Atom 31:Atom
32:CLASS 33:CLASS

=> d ide L33

L33 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 741672-69-5 REGISTRY
ED Entered STN: 09 Sep 2004
CN ***Propanediamide, N-(5-benzoyl-2,3,4,5-tetrahydro-1-methyl-2-oxo-1H-1,5-benzodiazepin-3-yl)-N'-[(3,5-difluorophenyl)methyl]-2-methyl- (9CI)***
(CA INDEX NAME)
MF C28 H26 F2 N4 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> => file marpat
FILE 'MARPAT' ENTERED AT 13:57:06 ON 02 MAY 2007
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FILE CONTENT: 1961-PRESENT VOL 146 ISS 18 (20070427/ED)

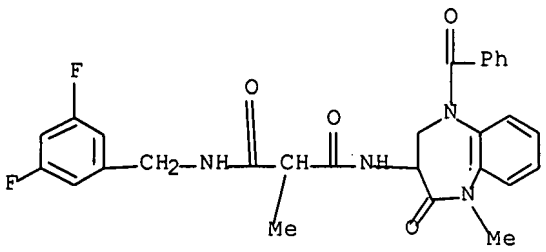
SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US	2007060644	15 MAR 2007
DE	102006023116	15 MAR 2007
EP	1762248	14 MAR 2007
JP	2007059877	08 MAR 2007
WO	2007030662	15 MAR 2007
GB	2429975	14 MAR 2007
FR	2890657	16 MAR 2007
RU	2295953	27 MAR 2007
CA	2556850	24 FEB 2007

Expanded G-group definition display now available.

=> d stat que L38
L34 STR



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Structure attributes must be viewed using STN Express query preparation.
L37           2 SEA FILE=MARPAT SSS FUL L34
L38           1 SEA FILE=MARPAT ABB=ON  PLU=ON  L37/COM


=> d ibib abs qhit L38 1

L38  ANSWER 1 OF 1  MARPAT  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         141:206827  MARPAT  Full-text
TITLE:                    Preparation of malonamides and related compounds as
                          γ-secretase inhibitors for the treatment of
                          Alzheimer's disease.
INVENTOR(S):              Galley, Guido; Goergler, Annick; Jacobsen, Helmut;
                          Kitas, Eric Argirios; Peters, Jens-Uwe
PATENT ASSIGNEE(S):       F. Hoffmann-La Roche A.-G., Switz.
SOURCE:                   PCT Int. Appl., 85 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE,
             BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU,
             MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN,
             GQ, GW, ML, MR, NE, SN, TD, TG
     AU 2004210036      A1   20040819       AU 2004-210036   20040127
     CA 2514267         A1   20040819       CA 2004-2514267  20040127
     EP 1592684         A1   20051109       EP 2004-705404   20040127
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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     BR 2004007262      A    20060131       BR 2004-7262     20040127
     CN 1745076         A    20060308       CN 2004-80003305 20040127
     JP 2006516556      T    20060706       JP 2006-500017   20040127
     US 2004220222      A1   20041104       US 2004-767784   20040129
     NO 2005003627      A    20050810       NO 2005-3627     20050726
PRIORITY APPLN. INFO.:                       EP 2003-2190     20030204
                                             WO 2004-EP674    20040127

GI
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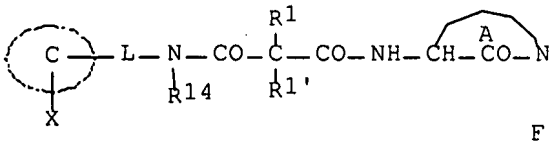

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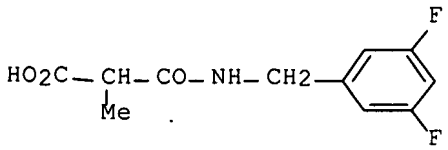
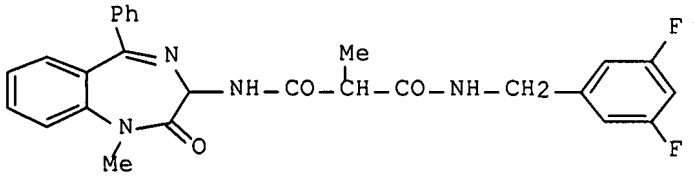


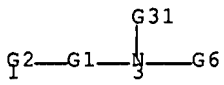
II



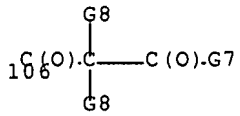
III

AB Title compds. I [L = bond, (CH2)1-2, CH(CH3), etc.; C = cyclic ring, e.g., Ph, pyridinyl, furanyl, etc.; X = (R2)1,2,3; (R2)1,2,3 = H, OH, halo, etc.; R1, R1' = H, alkyl, halo, etc.; R14 = H, alkyl, (CH2)2OH, etc.; A = substituted 5,7-dihydro-6H-dibenz[b,d]azepin-6-ones, 1,3-dihydro-5-phenyl- 1,4-benzodiazepin-2-ones, 3,4-dihydro-2-quinolinones, etc.] and their pharmaceutically acceptable salts and formulations were prepared For example, coupling of 3-amino-1,3-dihydro-1-methyl-5-phenyl-2H-1,4- benzodiazepin-2-one and malonamic acid II, e.g., prepared from di-Et Me malonate in 3-steps, afforded malonamide III in 67% yield. In γ-secretase inhibition assays, 37-examples of compds. I exhibited IC50 values ranging from 0.003-0.11 μM, the IC50 value of malonamide III was 0.83 μM. Compds. I are claimed useful for the treatment of Alzheimer's disease.

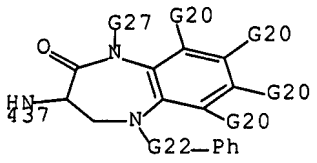
MSTR 1



G1 = CH2
G2 = Ph (opt. substd. by (1-3) G3)
G3 = F
G6 = 106



G7 = 437



G8 = alkyl <containing 1-6 C>
G22 = C(O)
G27 = Me
Patent location: claim 1
Note: and pharmaceutically suitable acid addition salts
Note: also incorporates claim 16
Note: substitution is restricted

=> => file registry
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DICTIONARY FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

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http://www.cas.org/support/stngen/stndoc/properties.html

=> file caplus
FILE 'CAPLUS' ENTERED AT 14:00:36 ON 02 MAY 2007
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PCL XL error

Subsystem: USERSTREAM

Error: MissingData

Operator: 0x0

Position: 0

PCL XL error

Subsystem: KERNEL

Error: StreamUndefined

Operator: 0x0

Position: 0

10/767784.
=> file registry
FILE 'REGISTRY' ENTERED AT 13:51:39 ON 02 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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STRUCTURE FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8
DICTIONARY FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

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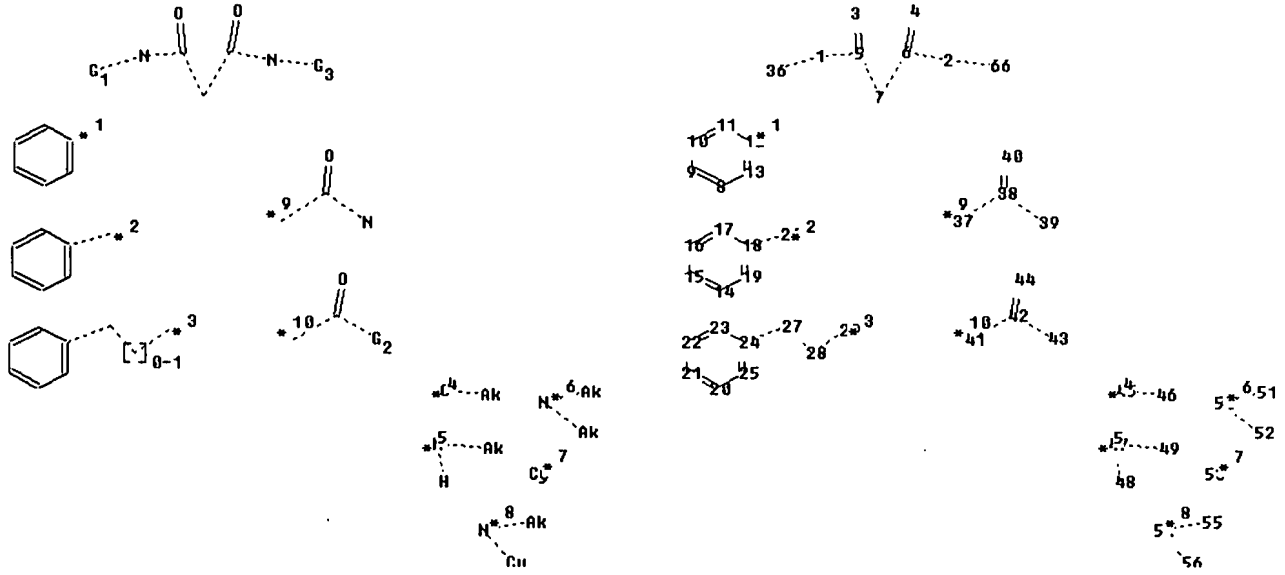
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

Uploading L1.str



chain nodes :
1 2 3 4 5 6 7 36 40 41 42 43 44 45 46 47 48 49 50 51 52 53
54 55 56 66
ring nodes :
8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 37 38 39

ring/chain nodes :

```
26  27  28  29
chain bonds :
1-5  1-36  2-6  2-66  3-5  4-6  5-7  6-7  18-26  24-27  38-40  41-42  42-43  42-44
45-46  47-48  47-49  50-51  50-52  54-55  54-56
ring/chain bonds :
27-28  28-29
ring bonds :
8-9  8-13  9-10  10-11  11-12  12-13  14-15  14-19  15-16  16-17  17-18  18-19  20-
21
20-25  21-22  22-23  23-24  24-25  37-38  38-39
exact/norm bonds :
1-5  1-36  2-6  2-66  3-5  4-6  5-7  6-7  18-26  24-27  27-28  28-29  37-38  38-39
38-40  41-42  42-43  42-44  45-46  47-48  47-49  50-51  50-52  54-55  54-56
normalized bonds :
8-9  8-13  9-10  10-11  11-12  12-13  14-15  14-19  15-16  16-17  17-18  18-19  20-
21
20-25  21-22  22-23  23-24  24-25


G1:[*1],[*2],[*3]

G2:[*4],[*5],[*6],[*7],[*8]

G3:[*9],[*10]

Match level :
1:CLASS  2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS  8:Atom  9:Atom
10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom
20:Atom  21:Atom
22:Atom  23:Atom  24:Atom  25:Atom  26:CLASS  27:CLASS  28:CLASS  29:CLASS
36:CLASS  37:Atom
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56:Atom  66:CLASS



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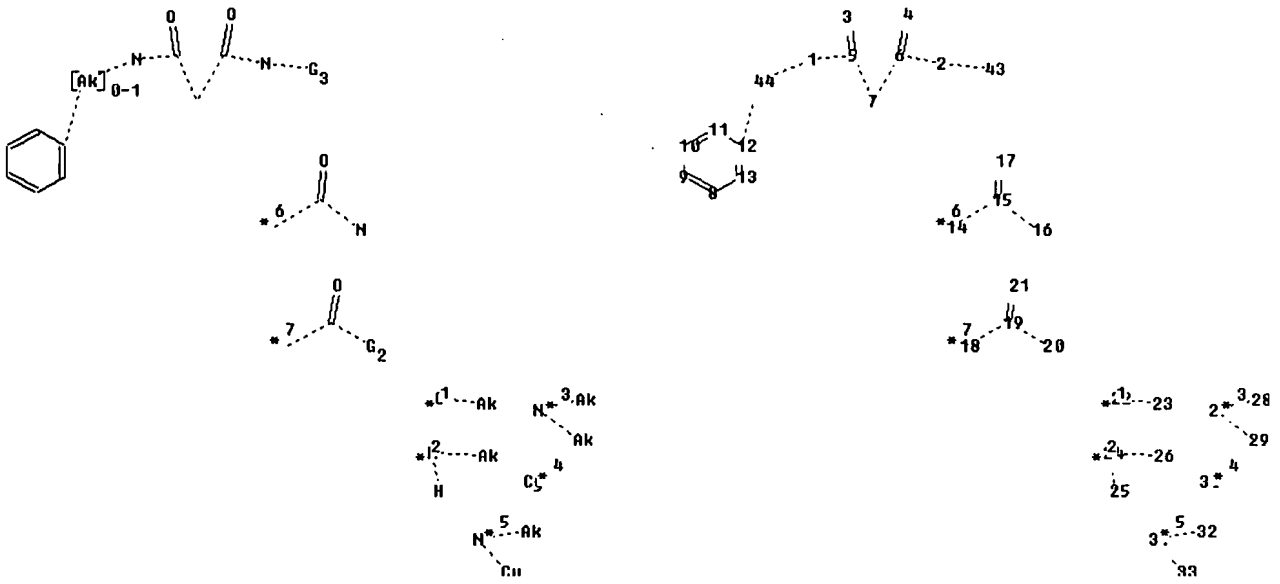

chain nodes :
1 2 3 4 5 6 7 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31
32 33 43 44
ring nodes :
8 9 10 11 12 13 14 15 16
chain bonds :
1-5 1-44 2-6 2-43 3-5 4-6 5-7 6-7 12-44 15-17 18-19 19-20 19-21 22-23
24-25 24-26 27-28 27-29 31-32 31-33
ring bonds :
8-9 8-13 9-10 10-11 11-12 12-13 14-15 15-16
exact/norm bonds :
1-5 1-44 2-6 2-43 3-5 4-6 5-7 6-7 12-44 14-15 15-16 15-17 18-19 19-20
19-21 22-23 24-25 24-26 27-28 27-29 31-32 31-33
normalized bonds :
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isolated ring systems :
containing 8 :

G2:[*1],[*2],[*3],[*4],[*5]

G3:[*6],[*7]

Connectivity :
44:2 E exact RC ring/chain
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom
10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS
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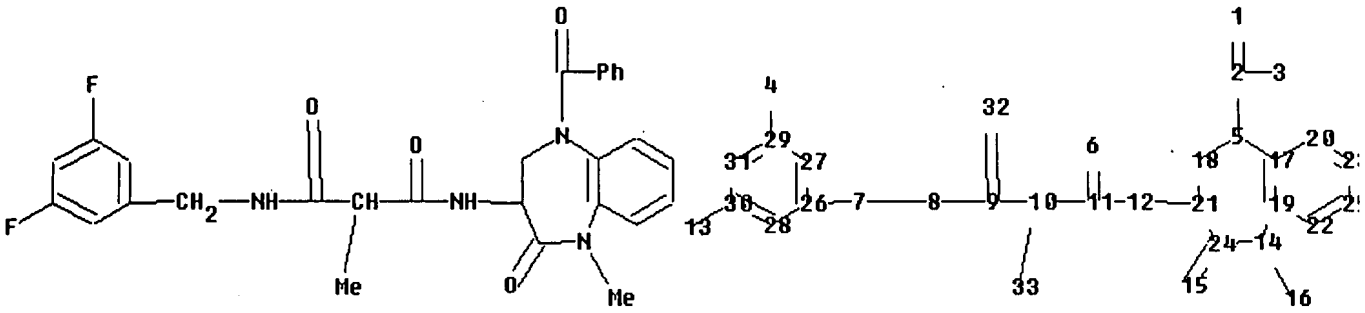

chain nodes :
1 2 3 4 6 7 8 9 10 11 12 13 15 16 32 33
ring nodes :
5 14 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31
chain bonds :
1-2 2-5 2-3 4-29 6-11 7-8 7-26 8-9 9-10 9-32 10-11 10-33 11-12 12-21
13-30 14-16 15-24
ring bonds :
5-17 5-18 14-19 14-24 17-19 17-20 18-21 19-22 20-23 21-24 22-25 23-25
26-27 26-28 27-29 28-30 29-31 30-31
exact/norm bonds :
1-2 2-5 5-17 5-18 6-11 8-9 9-32 11-12 12-21 14-19 14-24 15-24 18-21
21-24
exact bonds :
2-3 4-29 7-8 7-26 9-10 10-11 10-33 13-30 14-16
normalized bonds :
17-19 17-20 19-22 20-23 22-25 23-25 26-27 26-28 27-29 28-30 29-31 30-31

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:Atom 15:CLASS 16:CLASS 17:Atom 18:Atom
19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom
30:Atom 31:Atom
32:CLASS 33:CLASS

=> d ide L33

L33 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 741672-69-5 REGISTRY
ED Entered STN: 09 Sep 2004
CN *Propanediamide, N-(5-benzoyl-2,3,4,5-tetrahydro-1-methyl-2-oxo-1H-1,5-benzodiazepin-3-yl)-N'-[(3,5-difluorophenyl)methyl]-2-methyl- (9CI)*
(CA INDEX NAME)
MF C28 H26 F2 N4 O4
SR CA
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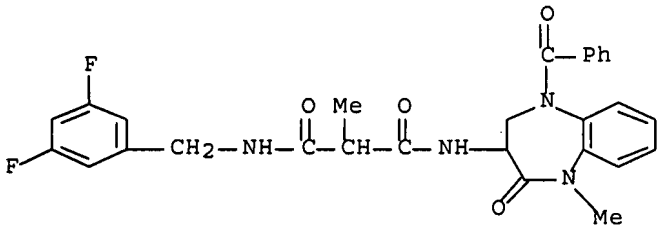

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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FILE 'MARPAT' ENTERED AT 13:57:06 ON 02 MAY 2007
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FILE CONTENT: 1961-PRESENT VOL 146 ISS 18 (20070427/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 2007060644 15 MAR 2007
DE 102006023116 15 MAR 2007
EP 1762248 14 MAR 2007
JP 2007059877 08 MAR 2007
WO 2007030662 15 MAR 2007
GB 2429975 14 MAR 2007
FR 2890657 16 MAR 2007
RU 2295953 27 MAR 2007
CA 2556850 24 FEB 2007

Expanded G-group definition display now available.

=> d stat que L38
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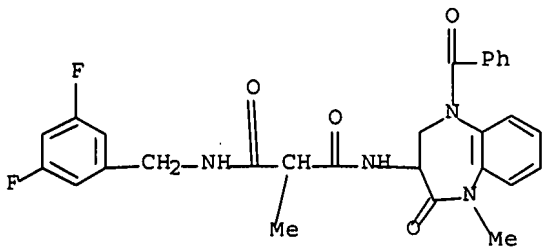

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L38  ANSWER 1 OF 1  MARPAT  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         141:206827  MARPAT  Full-text
TITLE:                    Preparation of malonamides and related compounds as
                          γ-secretase inhibitors for the treatment of
                          Alzheimer's disease.
INVENTOR(S):              Galley, Guido; Goergler, Annick; Jacobsen, Helmut;
                          Kitas, Eric Argirios; Peters, Jens-Uwe
PATENT ASSIGNEE(S):       F. Hoffmann-La Roche A.-G., Switz.
SOURCE:                   PCT Int. Appl., 85 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

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     EP 1592684         A1   20051109       EP 2004-705404   20040127
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     BR 2004007262      A    20060131       BR 2004-7262     20040127
     CN 1745076         A    20060308       CN 2004-80003305 20040127
     JP 2006516556      T    20060706       JP 2006-500017   20040127
     US 2004220222      A1   20041104       US 2004-767784   20040129
     NO 2005003627      A    20050810       NO 2005-3627     20050726
PRIORITY APPLN. INFO.:                      EP 2003-2190     20030204
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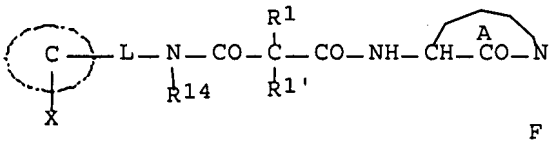

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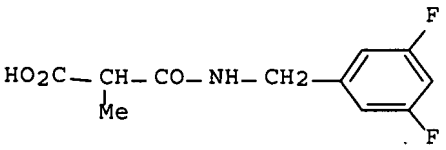

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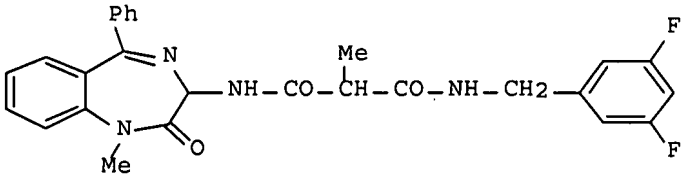
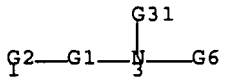


III

AB Title compds. I [L = bond, (CH2)1-2, CH(CH3), etc.; C = cyclic ring, e.g., Ph, pyridinyl, furanyl, etc.; X = (R2)1,2,3; (R2)1,2,3 = H, OH, halo, etc.; R1, R1' = H, alkyl, halo, etc.; R14 = H, alkyl, (CH2)2OH, etc.; A = substituted 5,7-dihydro-6H-dibenz[b,d]azepin-6-ones, 1,3-dihydro-5-phenyl- 1,4-benzodiazepin-2-ones, 3,4-dihydro-2-quinolinones, etc.] and their pharmaceutically acceptable salts and formulations were prepared For example, coupling of 3-amino-1,3-dihydro-1-methyl-5-phenyl-2H-1,4- benzodiazepin-2-one and malonamic acid II, e.g., prepared from di-Et Me malonate in 3-steps, afforded malonamide III in 67% yield. In γ-secretase inhibition assays, 37-examples of compds. I exhibited IC50 values ranging from 0.003-0.11 μM, the IC50 value of malonamide III was 0.83 μM. Compds. I are claimed useful for the treatment of Alzheimer's disease.

MSTR 1



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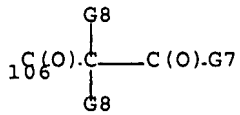
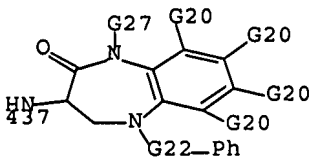
G2 = Ph (opt. substd. by (1-3) G3)
G3 = F
G6 = 106



G7 = 437



G8 = alkyl <containing 1-6 C>
G22 = C(O)
G27 = Me
Patent location: claim 1
Note: and pharmaceutically suitable acid addition salts
Note: also incorporates claim 16
Note: substitution is restricted

=> => file registry
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STRUCTURE FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8
DICTIONARY FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

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=> file caplus
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FILE LAST UPDATED: 1 May 2007 (20070501/ED)

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=> s (L16 or L48-L49)
L50           9 (L16 OR (L48 OR L49))

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L50  ANSWER 1 OF 9  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2007:175657  CAPLUS  Full-text
DOCUMENT NUMBER:          146:251750
TITLE:                    Preparation of fluoro substituted 2-oxo-azepan
                          derivatives as γ-secretase inhibitors
INVENTOR(S):              Flohr, Alexander; Galley, Guido;
                          Jakob-Roetne, Roland; Kitas, Eric Argirios;
                          Wostl, Wolfgang
PATENT ASSIGNEE(S):       Switz.
SOURCE:                   U.S. Pat. Appl. Publ., 18pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
     US 2007037789         A1    20070215    US 2006-500662          20060808
     WO 2007020190         A1    20070222    WO 2006-EP64935         20060802
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
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PRIORITY APPLN. INFO.: EP 2005-107455 A 20050812

OTHER SOURCE(S): MARPAT 146:251750

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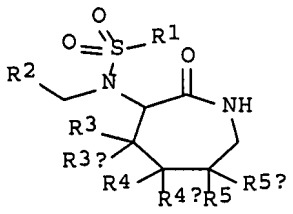

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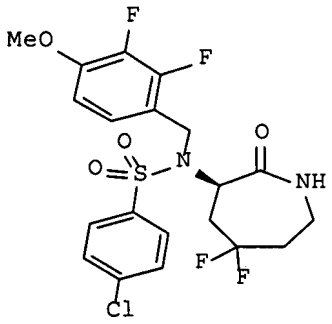

II

AB The title fluoro substituted 2-oxo-azepan derivs. I [wherein R1 = halogenated alkyl or (un)substituted (hetero)aryl; R2 = (un)substituted heterocycloalkyl or (hetero)aryl; R3/R3a, R4/R4a, and R5/R5a = independently H or F; wherein at least one of R4/R4a and R5/R5a = F], or pharmaceutically acceptable acid salts, optical enantiomers, racemates, or diastereomeric mixts. thereof were prepared as γ-secretase inhibitors for the treatment of Alzheimer's disease or common cancers including, but not limited to, cervical carcinomas, breast carcinomas, and malignancies of the hematopoietic system (no data). For example, 4-chloro-N-((R)-5,5- difluoro-2-oxo-azepan-3-yl)benzenesulfonamide (preparation given) was alkylated using 1-bromomethyl-2,3-difluoro-4-methoxybenzene to give II. II showed inhibitory activity with IC50 of 2 nM against γ-secretase. Formulations as tablets and capsules were described.

INCL 514212030; 540527000

CC 27-21 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63

L50 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:53048 CAPLUS Full-text

DOCUMENT NUMBER: 144:128869

TITLE: Preparation of N-(2-oxoazepan-3-yl)sulfonamides as γ-secretase inhibitors for treating Alzheimer's disease and cancers

INVENTOR(S): ***Galley, Guido; Kitas, Eric, Argirios*** ; Jakob-Roetne, Roland

PATENT ASSIGNEE(S): F. Hoffmann-La Roche AG, Switz.

SOURCE: PCT Int. Appl., 107 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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WO 2006005486	A1	20060119	WO 2005-EP7268		20050706
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CA 2573372	A1	20060119	CA 2005-2573372		20050706
EP 1768960	A1	20070404	EP 2005-754795		20050706
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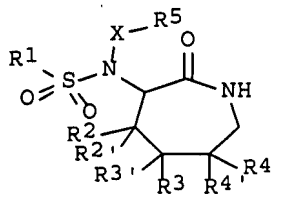
US 2006014945	A1	20060119	US 2005-179703		20050712
PRIORITY APPLN. INFO.:			EP 2004-103339	A	20040713
			WO 2005-EP7268	W	20050706
OTHER SOURCE(S):	MARPAT 144:128869				

GI



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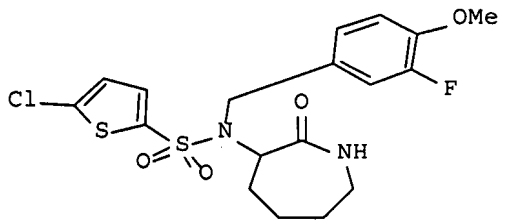

II

AB Title compds. I [R1 = (un)substituted hetero/aryl; R2-R4, R2'-R4' = H, lower alkyl, Ph or lower alkyl substituted by halogen; R5 = cycloalkyl, (un)substituted hetero/aryl; X = CHR; R = H, lower alkyl; and their pharmaceutically suitable acid addition salts, optical pure enantiomers, racemates or diastereomeric] were prepared as γ-secretase inhibitors. Thus, reductive amination of 3-fluoro-p-anisaldehyde with 3-aminoazepan-2-one and reaction with 5-chlorothiophene-2-sulfonyl chloride gave sulfonamide II. Preferred I inhibited γ-secretase with IC50 < 0.3 μM. I are useful in the treatment of Alzheimer's disease or common cancers.

IC ICM C07D223-08

ICS A61K031-55; A61P035-00; A61P025-28
CC 27-21 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:303395 CAPLUS Full-text
DOCUMENT NUMBER: 142:373708
TITLE: Preparation of carbamic acid alkyl ester derivatives as
INVENTOR(S): Flohr, Alexander; ***Galley, Guido***; Jakob-Roetne, Roland; ***Kitas, Eric Argirios***; ***Peters, Jens-Uwe***; Wostl, Wolfgang
PATENT ASSIGNEE(S): Hoffmann-La Roche Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 38 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2005075327	A1	20050407	US 2004-951229		20040927
US 7166587	B2	20070123			
AU 2004283803	A1	20050506	AU 2004-283803		20040927
CA 2541470	A1	20050506	CA 2004-2541470		20040927
WO 2005040126	A1	20050506	WO 2004-EP10821		20040927
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
EP 1673347	A1	20060628	EP 2004-787028		20040927
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR					
BR 2004015070	A	20061212	BR 2004-15070		20040927
CN 1894217	A	20070110	CN 2004-80033374		20040927
JP 2007507447	T	20070329	JP 2006-530028		20040927
NO 2006001469	A	20060626	NO 2006-1469		20060331
PRIORITY APPLN. INFO.:			EP 2003-22650	A	20031006
			WO 2004-EP10821	W	20040927

OTHER SOURCE(S): CASREACT 142:373708; MARPAT 142:373708
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The compds. of general formula (I) and (II) [R1 = each (un)substituted -(CHR')q-aryl or -(CHR')q-heteroaryl, lower alkyl, lower alkenyl, -(CH2)nSiMe3, -(CH2)n-O-lower alkyl, -(CH2)n-S-lower alkyl, -(CH2)q-cycloalkyl, or -(CH2)n-

[CH(OH)]m-(CF2)p-CHF(3-q), -(CH2)n-CR2-CF3 (wherein the two R radicals form together with the carbon atom a cycloalkyl ring); R' = H, lower alkyl; n = 1-3; m = 0, 1; p = 0-6; q = 0-3; R2 = H, lower alkyl; R3 = H, lower alkyl, -CH2CF2CF3, CH2CF3, (CH2)2CF3, CF3, CHF2, CH2F, (un)substituted aryl, -(CH2)nNR5R6 (wherein R5, R6 = H, lower alkyl); R4 = Q, Q1 (wherein R7 = H, lower alkyl, -(CH2)nCF3, -(CH2)n-cycloalkyl); R8 = H, lower alkyl, -COPh, -C(O)-lower alkyl, -C(O)O-(CH2)n-cycloalkyl, -C(O)O-(CH2)n-lower alkyl, -C(O)NH-(CH2)n-lower alkyl, -C(O)NH-(CH2)n-cycloalkyl; R9 = H, lower alkyl, -(CH2)n-cycloalkyl, -(CH2)n-CF3] or pharmaceutically acceptable salts, optically pure enantiomers, racemates or diastereomeric mixts. thereof are prepared These compds. inhibit amyloidogenic Abeta peptides, i.e. β-amyloid (Aβ) peptides, and are useful for the treatment of Alzheimer's disease. β-amyloid peptides. Thus, 0.12 g (0.25 mmol) carbonic acid 4-nitrophenyl ester (S)-1-((S)-6-oxo-6,7-dihydro-5H- dibenzo[b,d]azepin-7-ylcarbamoyl)ethyl ester and 543 μl 2,2,3,3,3.pentafluoropropylamine were stirred at room temperature over night to give, after silica gel chromatog., 0.075 g (63%) (2,2,3,3,3-pentafluoropropyl)carbamic acid (1S)-1-[((7S)-6-oxo-6,7-dihydro-5H-dibenzo[b,d]azepin-7-yl)carbamoyl]ethyl ester (III). III showed IC50 of 0.001 μM against γ-secretase.

IC ICM A61K031-5513
ICS A61K031-55; C07D243-24
INCL 514212040; X51-422.1; X54-050.8; X54-052.2
CC 27-21 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 28
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:220131 CAPLUS Full-text
DOCUMENT NUMBER: 142:298014
TITLE: Preparation of dibenzoazepinylmalonamides, dibenzooxepinylmalonamides, benzodiazepinylmalonamides, and related compounds as γ-secretase inhibitors for treatment of Alzheimer's disease.
INVENTOR(S): Flohr, Alexander; ***Galley, Guido***; Jakob-Roetne, Roland; ***Kitas, Eric Argirios***; ***Peters, Jens-Uwe***; Wostl, Wolfgang
PATENT ASSIGNEE(S): Hoffmann-La Rache Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 59 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005054633	A1	20050310	US 2004-933177	20040902
US 7160875	B2	20070109		
AU 2004270361	A1	20050317	AU 2004-270361	20040831
CA 2537440	A1	20050317	CA 2004-2537440	20040831
WO 2005023772	A1	20050317	WO 2004-EP9700	20040831

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

BR 2004013533	A	20061010	BR 2004-13533	20040831
EP 1711470	A1	20061018	EP 2004-764665	20040831
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1875005	A	20061206	CN 2004-80032641	20040831
JP 2007505063	T	20070308	JP 2006-525701	20040831
NO 2006001047	A	20060404	NO 2006-1047	20060303
PRIORITY APPLN. INFO.:			EP 2003-19683 A	20030909
			WO 2004-EP9700 W	20040831

OTHER SOURCE(S): MARPAT 142:298014

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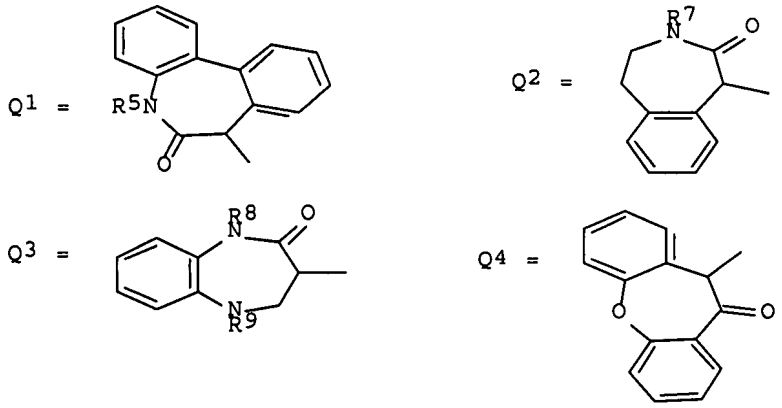

AB Malonamides R1NHCOCR3R4CONHR2 [R1= Q1-Q4; R2 = alkyl, alkynyl, alkylthio, alkoxy(alkyl), halo(alkyl), etc.; R3, R4 = H, alkyl, alkoxy, Ph, halo; R5 = H, alkyl, trifluoromethyl(alkyl), cycloalkyl(alkyl); R6 = H, halo; R7 = H, alkyl; R8 = H, alkyl, alkynyl, trifluoromethyl(alkyl), cycloalkyl(alkyl), (halo-substituted) phenyl(alkyl); R9 = H, alkyl, CHO, alkylcarbonyl, F3CCO, (substituted) PhCO, etc.], were prepared Thus, 2-methyl-N-(5-methyl-6-oxo-6,7-dihydro-5H-dibenzo[b,d]azepin-7- yl)malonamic acid (preparation given), cyclopropylmethylamine, and 2-(2-pyridon-1-yl)-1,1,3,3-tetramethyluronium tetrafluoroborate (TPTU) were shaken together overnight in DMF to give N-cyclopropylmethyl-2-methyl- N'-(5-methyl-6-oxo-6,7-dihydro-5H-dibenzo[b,d]azepin-7-yl)malonamide. The latter inhibited γ-secretase with IC50 = 0.09 μM.

IC ICM A61K031-55
ICS A61K031-5513; A61K031-335

INCL 514212040; X51-421.207; X51-422.1; X51-445.0; X54-050.9; X54-052.2; X54-052.3

CC 27-21 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 28, 63

IT 847927-01-9P 847927-02-0P 847927-03-1P 847927-04-2P 847927-05-3P
847927-06-4P 847927-07-5P 847927-08-6P 847927-09-7P 847927-10-0P
847927-11-1P 847927-12-2P 847927-13-3P 847927-14-4P

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847927-30-4P 847927-31-5P 847927-32-6P 847927-33-7P 847927-34-8P
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847927-51-9P 847927-52-0P 847927-53-1P 847927-54-2P 847927-55-3P
847927-56-4P 847927-57-5P 847927-58-6P 847927-59-7P 847927-60-0P
847927-61-1P 847927-62-2P 847927-63-3P 847927-64-4P 847927-65-5P
847927-66-6P 847927-67-7P 847927-68-8P 847927-69-9P 847927-70-2P
847927-71-3P 847927-72-4P 847927-73-5P 847927-74-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dibenzoazepinylmalonamides, dibenzooxepinylmalonamides, benzodiazepinylmalonamides, and related compds. as γ-secretase inhibitors for treatment of Alzheimer's disease)
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1019771 CAPLUS Full-text
DOCUMENT NUMBER: 142:6564
TITLE: Preparation of 1,4-benzoxazepin-3-ones as inhibitors of γ-secretase for the treatment of Alzheimer's disease
INVENTOR(S): ***Galley, Guido***; Goodnow, Robert Alan; ***Peters, Jens-Uwe***
PATENT ASSIGNEE(S): Hoffmann-La Roche Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 27 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004235819	A1	20041125	US 2004-838054	20040503
US 7060698	B2	20060613		
AU 2004238037	A1	20041125	AU 2004-238037	20040514
CA 2524640	A1	20041125	CA 2004-2524640	20040514
WO 2004100958	A1	20041125	WO 2004-EP5177	20040514
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1631296	A1	20060308	EP 2004-732944	20040514
EP 1631296	B1	20070425		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1794997	A	20060628	CN 2004-80014015	20040514
BR 2004010647	A	20060704	BR 2004-10647	20040514
JP 2007501261	T	20070125	JP 2006-529815	20040514

PRIORITY APPLN. INFO.: EP 2003-11040 A 20030519
WO 2004-EP5177 W 20040514

OTHER SOURCE(S): MARPAT 142:6564

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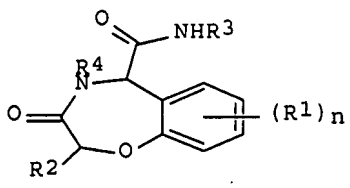

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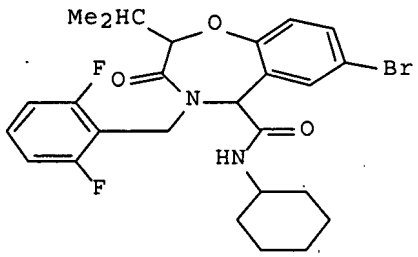

II

AB 1,4-Benzooxazepin-3-ones I [m = 0-2; n = 1, 2; p = 1, 2; R1 = H, halogen, alkoxy, amino, alkylamino, dialkylamino; R2 = H, alkyl, cycloalkyl-(CH2)m, Ph(CH2)m, alkoxy-(CH2)m; R3 = alkyl, alkoxycarbonyl-(CH2)m, Ph(CH2)m, cycloalkyl; R4 = (un)substituted Ph(CH2)p, cycloalkyl, tetrahydronaphthalen-1-yl, 9-fluorenyl, alkyl] such as II are prepared as γ-secretase inhibitors for the treatment of Alzheimer's disease. Treatment of 5-bromosalicylaldehyde with base followed by addition of Et 2-bromo-3-methylbutyrate yields Et 2-(4-bromo-2-formylphenoxy)-3- methylbutanoate, which is hydrolyzed to yield 2-(4-bromo-2-formylphenoxy)- 3-methylbutanoic acid (III); stirring III with 2,6-difluorobenzylamine and cyclohexyl isocyanide in DMSO yields II. IC50 values (without units) are given for the inhibition of γ-secretase by some of the title compds. E.g., II inhibits γ-secretase with an IC50 value of 0.28 (no units given). A process for the preparation of the title compds. using a cyclocondensation of (formylaryloxy)alkanoic acids, amines, and isonitriles is claimed.

IC ICM A61K031-553
ICS C07D413-02

INCL 514211050; X54-049.0

CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:675740 CAPLUS Full-text

DOCUMENT NUMBER: 141:206827

TITLE: Preparation of malonamides and related compounds as γ-secretase inhibitors for the treatment of Alzheimer's disease.

INVENTOR(S): ***Galley, Guido; Goergler, Annick; Jacobsen, Helmut; Kitas, Eric Argirios ; Peters, Jens-Uwe***

PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.

SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004069826	A1	20040819	WO 2004-EP674	20040127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004210036	A1	20040819	AU 2004-210036	20040127
CA 2514267	A1	20040819	CA 2004-2514267	20040127
EP 1592684	A1	20051109	EP 2004-705404	20040127
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2004007262	A	20060131	BR 2004-7262	20040127
CN 1745076	A	20060308	CN 2004-80003305	20040127
JP 2006516556	T	20060706	JP 2006-500017	20040127
US 2004220222	A1	20041104	US 2004-767784	20040129
NO 2005003627	A	20050810	NO 2005-3627	20050726
PRIORITY APPLN. INFO.:			EP 2003-2190 A	20030204
			WO 2004-EP674 W	20040127

OTHER SOURCE(S): MARPAT 141:206827

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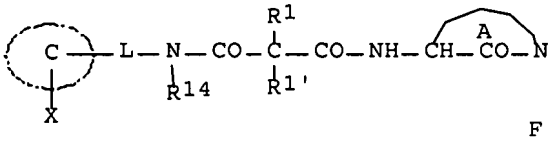

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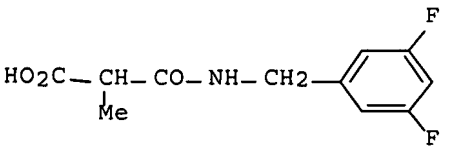
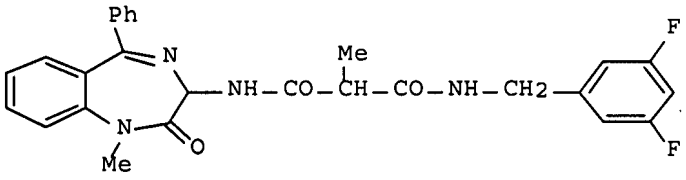


II



III

AB Title compds. I [L = bond, (CH2)1-2, CH(CH3), etc.; C = cyclic ring, e.g., Ph, pyridinyl, furanyl, etc.; X = (R2)1,2,3; (R2)1,2,3 = H, OH, halo, etc.; R1, R1' = H, alkyl, halo, etc.; R14 = H, alkyl, (CH2)2OH, etc.; A = substituted 5,7-dihydro-6H-dibenz[b,d]azepin-6-ones, 1,3-dihydro-5-phenyl- 1,4-benzodiazepin-2-ones, 3,4-dihydro-2-quinolinones, etc.] and their pharmaceutically acceptable salts and formulations were prepared For example, coupling of 3-amino-1,3-dihydro-1-methyl-5-phenyl-2H-1,4- benzodiazepin-2-one and malonamic acid II, e.g., prepared from di-Et Me malonate in 3-steps, afforded malonamide III in 67% yield. In γ-secretase inhibition assays, 37-

examples of compds. I exhibited IC50 values ranging from 0.003-0.11 μM, the IC50 value of malonamide III was 0.83 μM. Compds. I are claimed useful for the treatment of Alzheimer's disease.

IC ICM C07D401-06
ICS C07D217-06; C07D403-06; C07D471-08; C07D401-04; C07D471-04; C07D471-06; C07D209-44; C07D209-18; C07D223-18; C07D401-12; C07D405-12; C07D409-12; C07C237-12; C07C237-14

CC 23-18 (Aliphatic Compounds)
Section cross-reference(s): 1, 63

IT *741672-55-9P 741672-56-0P 741672-57-1P*
741672-58-2P 741672-59-3P 741672-60-6P
741672-61-7P 741672-62-8P 741672-63-9P
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741672-68-4P 741672-69-5P 741672-70-8P
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741673-79-0P 741673-80-3P 741673-81-4P
741673-82-5P 741673-83-6P 741673-84-7P
741673-85-8P 741673-86-9P 741673-87-0P
741673-88-1P 741673-89-2P 741673-90-5P
741673-91-6P 741673-92-7P 741673-93-8P
741673-94-9P 741673-95-0P 741673-96-1P
741673-97-2P 741673-98-3P 741673-99-4P
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741674-06-6P 741674-07-7P 741674-08-8P

741674-09-9P *741674-10-2P* *741674-11-3P*
741674-12-4P *741674-13-5P* *741674-14-6P*
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741674-21-5P *741674-22-6P* 741674-23-7P 741674-24-8P
741674-25-9P 741674-26-0P 741674-27-1P 741674-28-2P
741674-29-3P *741674-30-6P* *741674-31-7P*
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741674-40-8P *741674-99-7P*
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of malonamides and related compds. as γ-secretase inhibitors for the treatment of Alzheimer's disease.)

IT 2985-33-3P, 2-Methylmalonic acid monoethyl ester 119860-05-8P
741674-41-9P 741674-42-0P 741674-44-2P 741674-45-3P 741674-46-4P
741674-47-5P 741674-48-6P 741674-49-7P *741674-50-0P*
741674-51-1P 741674-54-4P 741674-55-5P 741674-56-6P 741674-57-7P
741674-58-8P 741674-59-9P, N-(3,5-Difluorobenzyl)malonamic acid
741674-60-2P 741674-64-6P 741674-65-7P 741674-66-8P 741674-67-9P
741674-68-0P 741674-69-1P 741674-70-4P 741674-71-5P 741674-72-6P
741674-73-7P 741674-74-8P 741674-75-9P 741674-78-2P 741674-79-3P
741674-81-7P 741674-82-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of malonamides and related compds. as γ-secretase inhibitors for the treatment of Alzheimer's disease.)

L50 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:888744 CAPLUS Full-text
DOCUMENT NUMBER: 137:384847
TITLE: 1-Oxa-3,9-diazaspiro[5,5]undecan-2-ones as antagonists of the neurokinin receptor
INVENTOR(S): Cai, Hai-Ying; Dillon, Michael Patrick; ***Galley, Guido***; ***Goergler, Annick***; Kolczewski, Sabine; Muszynski-Barsy, Dawn Marie
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

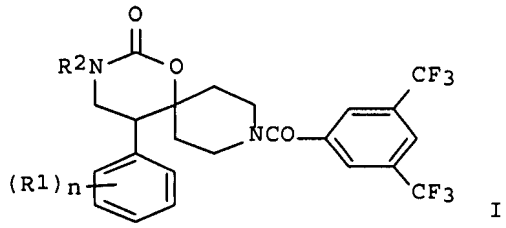
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002092604	A1	20021121	WO 2002-EP4935	20020506
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2447329	A1	20021121	CA 2002-2447329	20020506
AU 2002342238	A1	20021125	AU 2002-342238	20020506
EP 1390372	A1	20040225	EP 2002-742943	20020506

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

BR 2002009604	A	20040323	BR 2002-9604		20020506
CN 1507449	A	20040623	CN 2002-809473		20020506
JP 2004534758	T	20041118	JP 2002-589488		20020506
US 2003004163	A1	20030102	US 2002-143431		20020510
US 6599900	B2	20030729			
ZA 2003008535	A	20050131	ZA 2003-8535		20031031
PRIORITY APPLN. INFO.:			EP 2001-111644	A	20010514
			WO 2002-EP4935	W	20020506

OTHER SOURCE(S): MARPAT 137:384847

GI



I

AB Title compds. I [R1 = halogen, alkyl, alkoxy; R2 = H, alkyl, haloalkyl, OH, hydroxyalkyl, amino, aminoalkykl, alkoxyalkyl, carbamoylalkyl, heteroaryl, heteroarylalkyl, heterocyclic, heterocyclylalkyl; n = 0-2] were prepared for use as NK-1 antagonists. Thus, 3-ClC6H4CH2CN was treated with 1-[3,5-bis(trifluoromethyl)benzoyl]-4-piperidinone and cyclized with carbonyldiimidazole to give I [R1 = 3-Cl, R2 = H] which had a pKi for the NK-1 receptor of 8.29.

IC ICM C07D498-10
ICS A61K031-535

CC 28-13 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:904170 CAPLUS Full-text
DOCUMENT NUMBER: 136:37519
TITLE: Synthesis and use of triazaspirodecanone derivatives as neurokinin receptor antagonists
INVENTOR(S): ***Galley, Guido***; Godel, Thierry; ***Goergler, Annick***; Hoffmann, Torsten; Kolczewski, Sabine; Roever, Stephan
PATENT ASSIGNEE(S): F. Hoffmann-La Roche AG, Switz.
SOURCE: PCT Int. Appl., 90 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2001094346	A1	20011213	WO 2001-EP6305		20010601
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CU, CZ, DE, DK, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
US 2002006932	A1	20020117	US 2001-861795		20010521
US 6482829	B2	20021119			
CA 2411716	A1	20011213	CA 2001-2411716		20010601
EP 1292596	A1	20030319	EP 2001-945242		20010601
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
BR 2001011538	A	20030701	BR 2001-11538		20010601
JP 2003535863	T	20031202	JP 2002-501895		20010601
ZA 2002009488	A	20040223	ZA 2002-9488		20021121
PRIORITY APPLN. INFO.:			EP 2000-112285	A	20000608
			WO 2001-EP6305	W	20010601

OTHER SOURCE(S): MARPAT 136:37519
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = H, alkyl, alkenyl, Ph, (CH2)m-non aromatic heterocyclyl, (CH2)m-heteroaryl, (CH2)m-carboxamide, (CH2)m-C(O)alkyl, etc.; R2 = H, alkyl, halo, alkoxy; R3 = alkyl, alkoxy, halo, CF3; X = N-, C:, CH; X1/X2 = H, OH, alkoxy or may be together an oxo group; Y1/Y2 = H, alkyl, (CH2)m-Ph or may be together an oxo group; Z = bond, CH2, C(O); m = 0 - 4; n = 2 - 3; p = 0 - 2] were prepared Over 160 synthetic examples were disclosed. For example, 8-(3,5-bistrifluoromethylbenzoyl)-1-phenyl-1,3,8- triazaspiro[4.5]decan-4-one was reacted with 2-chloro-4,6-dimethoxy-1,3,5- triazine (1,2-dimethoxyethane, NaH, 100°C, 1 h) to give II. II had pKi = 8.66 for the NK-1 receptor. I are useful in the treatment of diseases related to NK-1 receptor antagonists.

IC ICM C07D471-10
ICS A61K031-445; C07D471-10; C07D239-00; C07D221-00

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

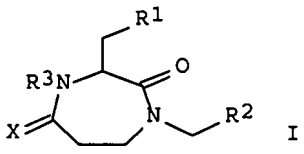
L50 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	2001:868429 CAPLUS Full-text
DOCUMENT NUMBER:	136:6018
TITLE:	1,4-Diazepan-2,5-dione derivatives and their use as NK-1 receptor antagonists
INVENTOR(S):	***Galley, Guido; Goergler, Annick***; Godel, Thierry; Heck, Reinhard
PATENT ASSIGNEE(S):	F. Hoffmann-La Roche A.-G., Switz.
SOURCE:	PCT Int. Appl., 38 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001090083	A1	20011129	WO 2001-EP5723	20010518
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CU, CZ, DE, DK, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002010174	A1	20020124	US 2001-854885	20010514
US 6452001	B2	20020917		
CA 2409842	A1	20011129	CA 2001-2409842	20010518
EP 1296961	A1	20030402	EP 2001-960225	20010518
EP 1296961	B1	20070214		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001011062	A	20030610	BR 2001-11062	20010518
JP 2003534332	T	20031118	JP 2001-586272	20010518
AT 353881	T	20070315	AT 2001-960225	20010518
ZA 2002008940	A	20040204	ZA 2002-8940	20021104
PRIORITY APPLN. INFO.:			EP 2000-111249 A	20000525
			WO 2001-EP5723 W	20010518

OTHER SOURCE(S): MARPAT 136:6018
GI



I

AB Title compds. I [R1, R2 = (un)substituted aryl, heteroaryl; R3 = H, alkyl, aminoalkyl, etc.; X = O, alkylimino, aminoalkylimino, etc.] were prepared for treatment of diseases related to the NK-1 receptor. Thus, I [R1 = 3,4-dichlorophenyl, R2 = 3,5-bis(trifluoromethyl)phenyl, R3 = H, X = O] was prepared in 3 steps starting from tert-Bu acrylate and 3,5-bis(trifluoromethyl)benzylamine. The affinities (pKi) of I for the NK-1 receptor were in the 8.00-9.00 range.

IC ICM C07D243-08
ICS A61K031-551; C07D487-04; A61K031-5517; C07D401-14; C07D403-06; C07D401-06; A61P029-00; A61P025-00; A61P013-10; A61P001-08

CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> file registry

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DICTIONARY FILE UPDATES:    1 MAY 2007  HIGHEST RN 934050-43-8

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FILE LAST UPDATED: 1 May 2007  (20070501/ED)

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http://www.cas.org/infopolicy.html
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=> d stat que L8
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L3          527 SEA FILE=REGISTRY SSS FUL L1
L7            4 SEA FILE=REGISTRY ABB=ON  PLU=ON  L3 AND C3/ESS
L8            3 SEA FILE=CAPLUS ABB=ON  PLU=ON  L7
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=> d stat que L26
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L3          527 SEA FILE=REGISTRY SSS FUL L1
L9              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L12         370 SEA FILE=REGISTRY SUB=L3 SSS FUL L9
L24           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  146420-49-7
L25         369 SEA FILE=REGISTRY ABB=ON  PLU=ON  L12 NOT L24
L26          65 SEA FILE=CAPLUS ABB=ON  PLU=ON  L25


=> s (L8 or L26) not L50
L53          64 (L8 OR L26) NOT L50

=> d ibib abs hitstr L53 1-64

L53  ANSWER 1 OF 64  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2007:190950  CAPLUS  Full-text
DOCUMENT NUMBER:          146:206636
TITLE:                    Novel malonic acid derivatives, processes for their
                          preparation, their use and pharmaceutical compositions
                          containing them (inhibition of factor Xa activity)
INVENTOR(S):              Defossa, Elisabeth; Heinelt, Uwe; Klingler, Otmar;
                          Zoller, Gerhard; Matter, Hans; Al-Obeidi, Fahad A.;
                          Walser, Armin; Wildgoose, Peter
PATENT ASSIGNEE(S):       Hoechst Marion Roussel Deutschland GmbH, Germany
SOURCE:                   PCT Int. Appl., 130pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   2
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    --------------------     --------
     WO 2000040571         A1    20000713    WO 1999-EP10340          19991223
         W:  AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
             CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
             MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
             SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     EP 1016663            A1    20000705    EP 1999-100002           19990102
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     CA 2358578            A1    20000713    CA 1999-2358578          19991223
     BR 9916732            A     20010925    BR 1999-16732            19991223
     EP 1140878            A1    20011010    EP 1999-964667           19991223
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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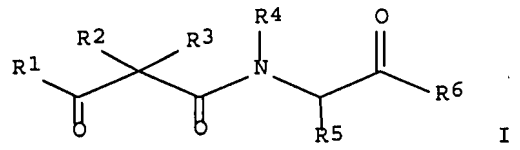
IE, SI, LT, LV, FI, RO

JP 2002534420	T	20021015	JP 2000-592279		19991223
NO 2001002983	A	20010615	NO 2001-2983		20010615
IN 2001CN00908	A	20050304	IN 2001-CN908		20010628
PRIORITY APPLN. INFO.:			EP 1999-100002	A	19990102
			EP 1999-119537	A	19991001
			WO 1999-EP10340	W	19991223

OTHER SOURCE(S): MARPAT 146:206636

GI



I

AB The present invention relates to the preparation of new compds. for the inhibition of blood clotting proteins, and more particularly, to malonic acid derivs., I (R1 = organo-amino, organo-alkoxy, etc.; R2 = H, C1-4 alkyl; R3 = (un)substituted C6-10-aryl-C1-4-alkyl; R4 = H, C1-4-alkyl, C3-7-cycloalkyl, C3-7-cycloalkyl-C1-4-alkyl, C6-10-aryl-C1-4-alkyl; R5 = H, C1-10-alkyl, C3-7-cycloalkyl, C3-7-cycloalkyl-C1-4-alkyl, C6-10-aryl, C6-10-aryl-C1-4-alkyl, etc.; R4R5 = cyclic hydrocarbyl; R6 = organo-alkoxy, organo-amino, etc.). Thus, 2-(R,S)-(4-carbamimidoylbenzyl)- N-[(S)-cyclohexyl(piperidin-4-yl-carbamoyl)methyl]-N',N'- dimethylmalonamide acetic acid salt was prepared in several steps starting from 2,2-dimethyl[1,3]dioxane-4,6-dione and 4-formyl-benzonitrile. I are inhibitors (Ki = 0.001 - 5.23 μM) of the blood clotting enzyme factor Xa. The invention also relates to processes for the preparation of I, to methods of inhibiting factor Xa activity and of inhibiting blood clotting, to the use of I in the treatment and prophylaxis of diseases, which can be treated or prevented by the inhibition of factor Xa activity such as thromboembolic diseases, and to the use of the compds. I in the preparation of medicaments to be applied in such diseases.

IT ***280553-80-2P 280553-83-5P 280553-85-7P***
280553-87-9P 280553-91-5P 280553-96-0P
280554-05-4P 280554-33-8P 280554-35-0P
280554-36-1P 280554-37-2P 923294-55-7P
923294-56-8P 923294-57-9P 923294-58-0P
923294-59-1P 923586-00-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of malonic acid derivs. as factor Xa inhibitors and anticoagulant agents)

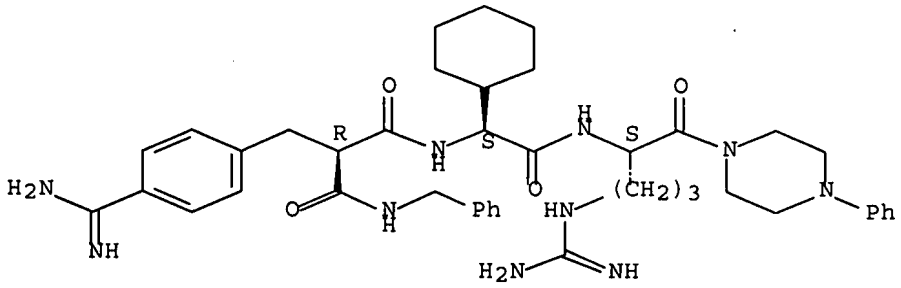
RN 280553-80-2 CAPLUS

CN Glycinamide, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(4-phenyl-1-piperazinyl)carbonyl]butyl]-2-cyclohexyl-, (2S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

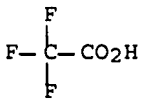
CRN 280553-79-9
CMF C42 H56 N10 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

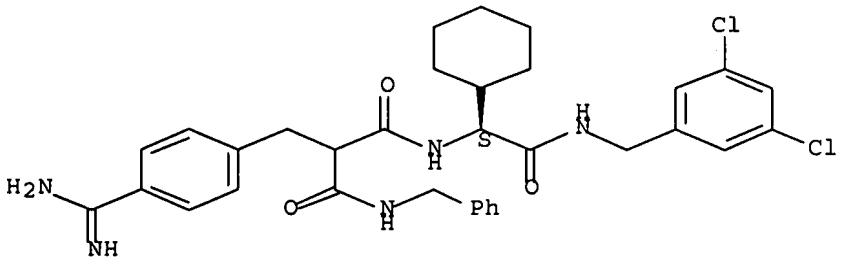


RN 280553-83-5 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-1-cyclohexyl-2-[[(3,5-dichlorophenyl)methyl]amino]-2-oxoethyl]-N'-(phenylmethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

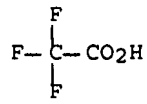
CRN 280553-82-4
CMF C33 H37 Cl2 N5 O3

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

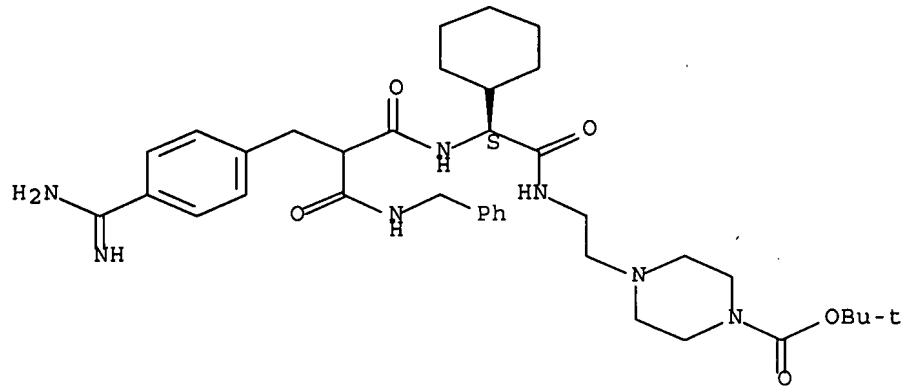


RN 280553-85-7 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[2-[[(2S)-[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]cyclohexylacetyl]amino]ethyl]-, 1,1-dimethylethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

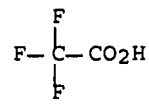
CRN 280553-84-6
CMF C37 H53 N7 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

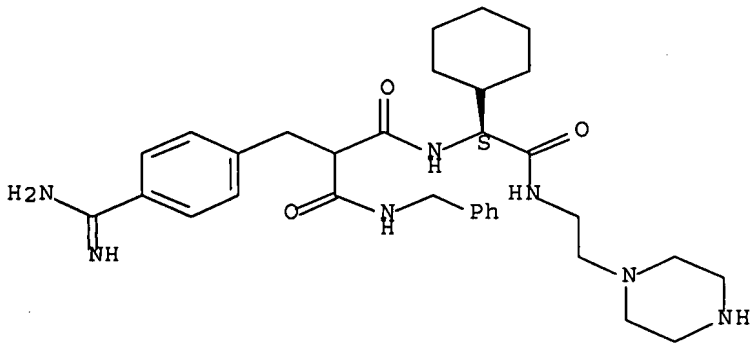


RN 280553-87-9 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-1-cyclohexyl-2-oxo-2-[[2-(1-piperazinyl)ethyl]amino]ethyl]-N'-(phenylmethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

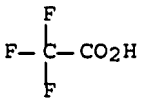
CRN 280553-86-8
CMF C32 H45 N7 O3

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

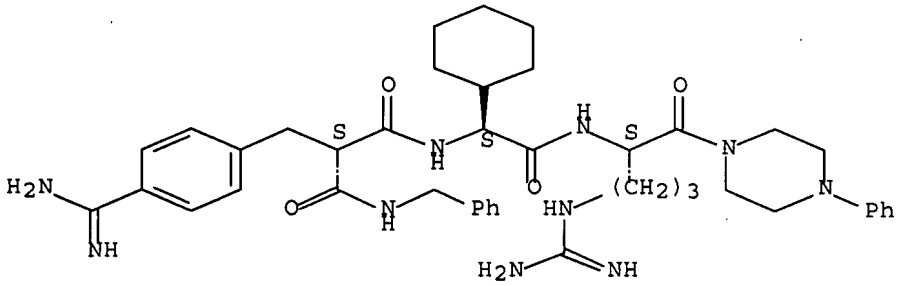


RN 280553-91-5 CAPLUS
CN Glycinamide, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(4-phenyl-1-piperazinyl)carbonyl]butyl]-2-cyclohexyl-, (2S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

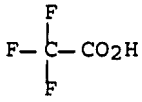
CRN 280553-90-4
CMF C42 H56 N10 O4

Absolute stereochemistry.



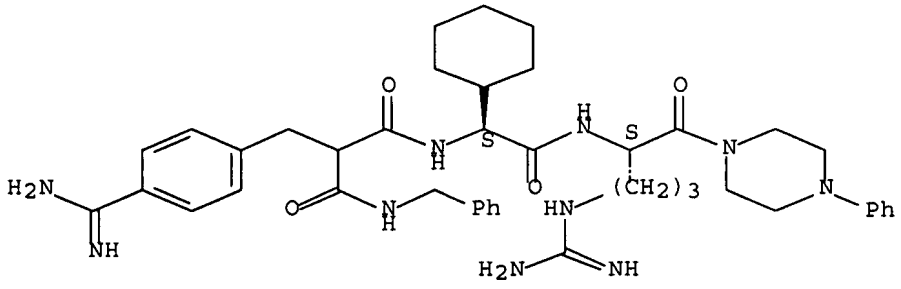
CM 2

CRN 76-05-1
CMF C2 H F3 O2



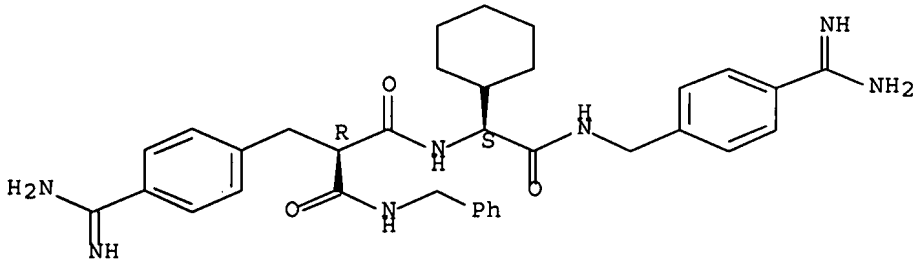
RN 280553-96-0 CAPLUS
CN Glycinamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(4-phenyl-1-piperazinyl)carbonyl]butyl]-2-cyclohexyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 280554-05-4 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-2-[[[4-(aminoiminomethyl)phenyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N'-(phenylmethyl)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

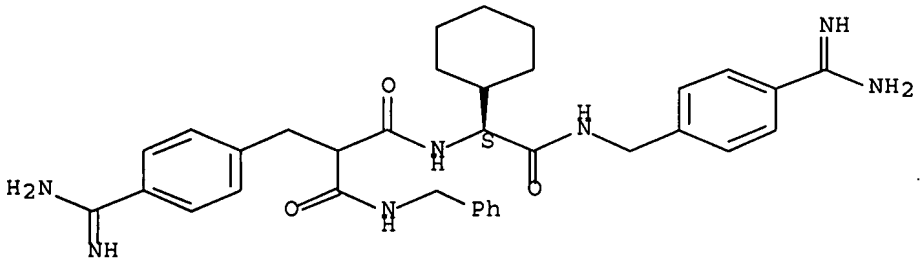


RN 280554-33-8 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-2-[[[4-(aminoiminomethyl)phenyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N'-(phenylmethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

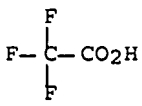
CRN 280554-32-7
CMF C34 H41 N7 O3

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

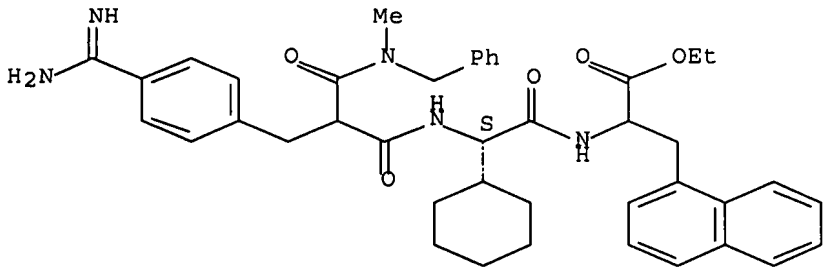


RN 280554-35-0 CAPLUS
CN Alanine, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-3-(1-naphthalenyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

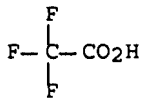
CRN 280554-34-9
CMF C42 H49 N5 O5

Absolute stereochemistry.



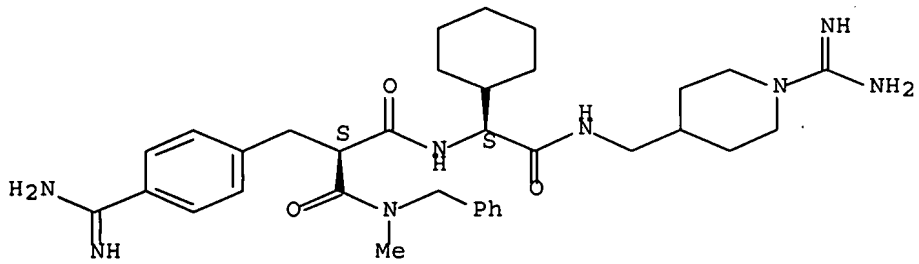
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 280554-36-1 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N'-[(1S)-2-[[[1-(aminoiminomethyl)-4-piperidinyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N-methyl-N-(phenylmethyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



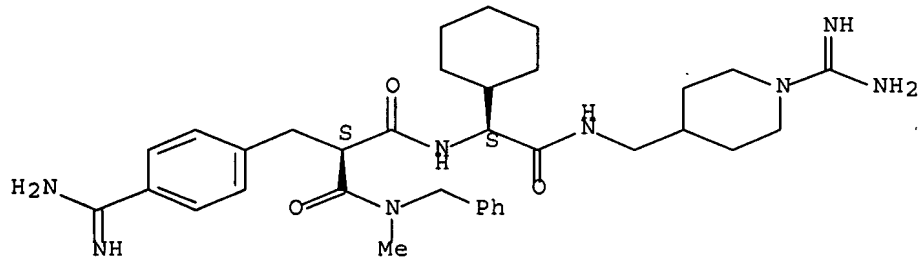
RN 280554-37-2 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N'-[(1S)-2-[[[1-(aminoiminomethyl)-4-piperidinyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N-

methyl-N-(phenylmethyl)-, (2S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

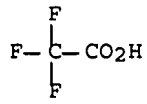
CRN 280554-36-1
CMF C34 H48 N8 O3

Absolute stereochemistry.



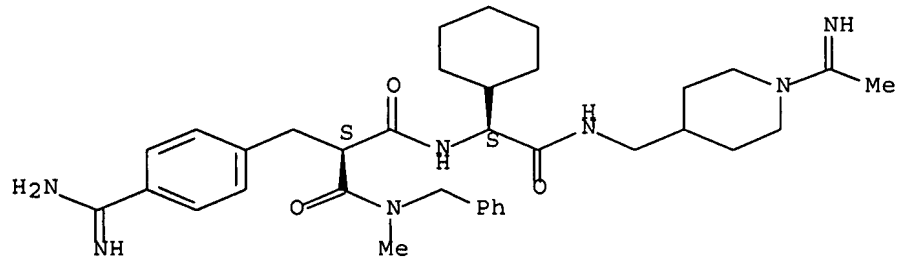
CM 2

CRN 76-05-1
CMF C2 H F3 O2



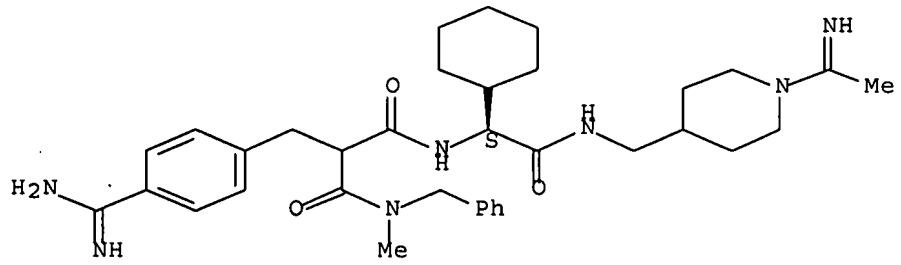
RN 923294-55-7 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N3-[(1S)-1-cyclohexyl-2-[[[1-(1-iminoethyl)-4-piperidinyl]methyl]amino]-2-oxoethyl]-N1-methyl-N1-(phenylmethyl)-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



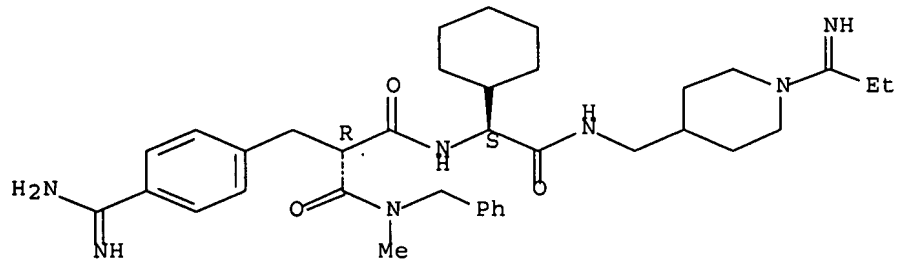
RN 923294-56-8 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N3-[(1S)-1-cyclohexyl-2-[[[1-(1-iminoethyl)-4-piperidinyl]methyl]amino]-2-oxoethyl]-N1-methyl-N1-(phenylmethyl)- (CA INDEX NAME)

Absolute stereochemistry.



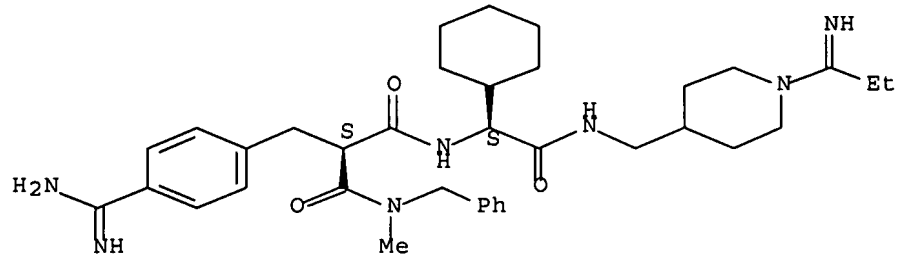
RN 923294-57-9 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N3-[(1S)-1-cyclohexyl-2-[[[1-(1-iminopropyl)-4-piperidinyl]methyl]amino]-2-oxoethyl]-N1-methyl-N1-(phenylmethyl)-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



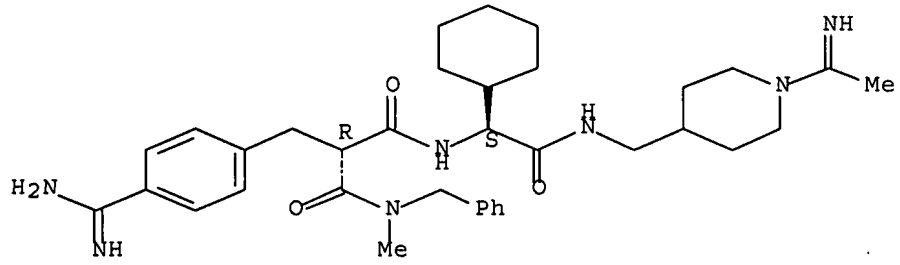
RN 923294-58-0 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N3-[(1S)-1-cyclohexyl-2-[[[1-(1-iminopropyl)-4-piperidinyl]methyl]amino]-2-oxoethyl]-N1-methyl-N1-(phenylmethyl)-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



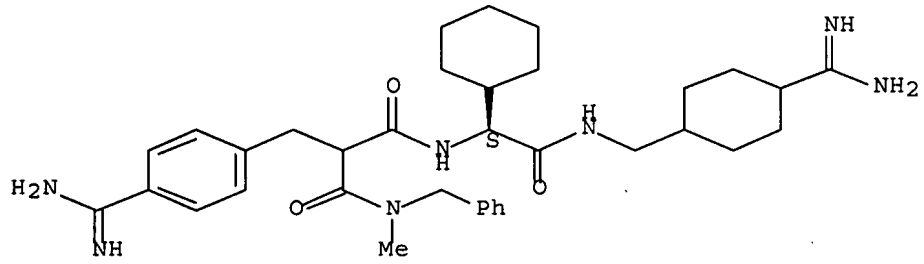
RN 923294-59-1 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N3-[(1S)-1-cyclohexyl-2-[[[1-(1-iminoethyl)-4-piperidinyl]methyl]amino]-2-oxoethyl]-N1-methyl-N1-(phenylmethyl)-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 923586-00-9 CAPLUS
CN Propanediamide, N3-[(1S)-2-[[[4-(aminoiminomethyl)cyclohexyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-2-[[4-(aminoiminomethyl)phenyl]methyl]-N1-methyl-N1-(phenylmethyl)- (CA INDEX NAME)

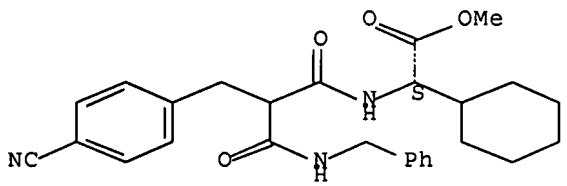
Absolute stereochemistry.



IT *280554-59-8P 280554-60-1P 280554-61-2P*
356545-90-9P 923294-54-6P 923585-99-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of malonic acid derivs. as factor Xa inhibitors and anticoagulant agents)

RN 280554-59-8 CAPLUS
CN Cyclohexaneacetic acid, α-[[2-[(4-cyanophenyl)methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

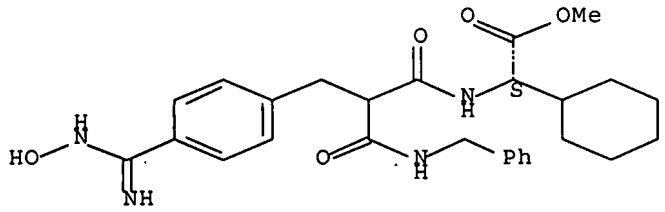
Absolute stereochemistry.



RN 280554-60-1 CAPLUS

CN Cyclohexaneacetic acid, α-[[2-[[4-[(hydroxyamino)iminomethyl]phenyl] methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

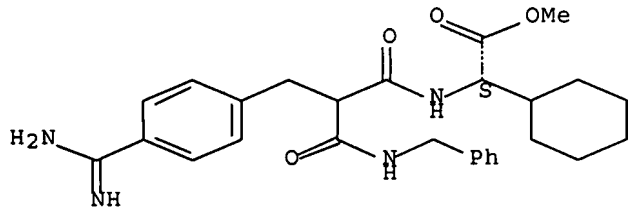
Absolute stereochemistry.



RN 280554-61-2 CAPLUS

CN Cyclohexaneacetic acid, α-[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

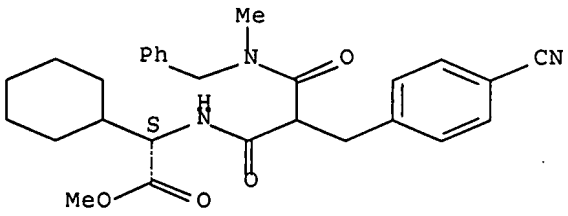
Absolute stereochemistry.



RN 356545-90-9 CAPLUS

CN Cyclohexaneacetic acid, α-[[2-[(4-cyanophenyl)methyl]-3-[methyl(phenylmethyl)amino]-1,3-dioxopropyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

Absolute stereochemistry.

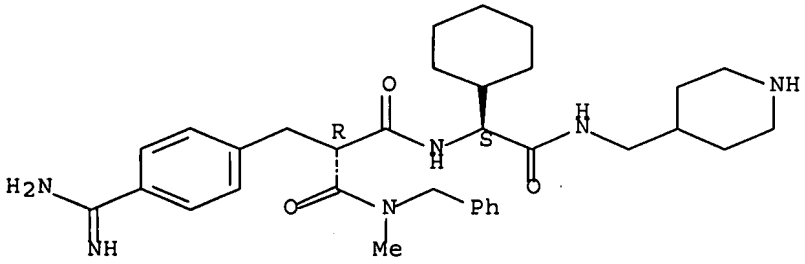


RN 923294-54-6 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N3-[(1S)-1-cyclohexyl-2-oxo-2-[(4-piperidinylmethyl)amino]ethyl]-N1-methyl-N1-(phenylmethyl)-, (2R)-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

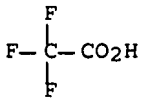
CRN 923294-53-5
CMF C33 H46 N6 O3

Absolute stereochemistry.



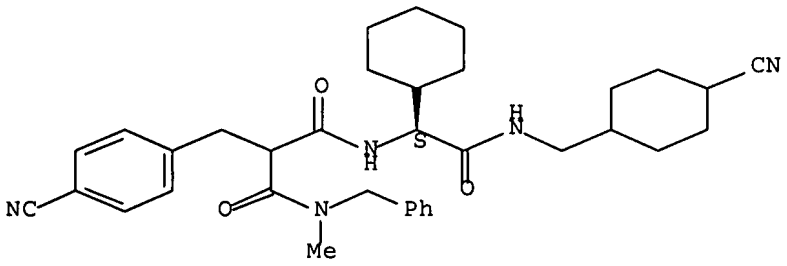
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 923585-99-3 CAPLUS
CN Propanediamide, N3-[(1S)-2-[[(4-cyanocyclohexyl)methyl]amino]-1-cyclohexyl-2-oxoethyl]-2-[(4-cyanophenyl)methyl]-N1-methyl-N1-(phenylmethyl)- (CA INDEX NAME)

Absolute stereochemistry.

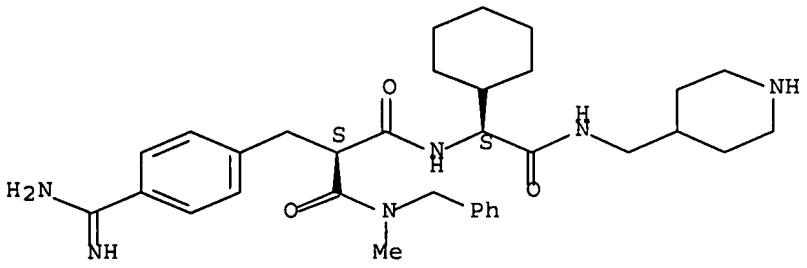


IT *923294-52-4P*
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of malonic acid derivs. as factor Xa inhibitors and anticoagulant agents)
RN 923294-52-4 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N3-[(1S)-1-cyclohexyl-2-oxo-2-[(4-piperidinylmethyl)amino]ethyl]-N1-methyl-N1-(phenylmethyl)-, (2S)-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

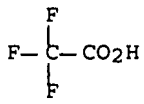
CRN 923294-51-3
CMF C33 H46 N6 O3

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS

L53 ANSWER 2 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:544815 CAPLUS Full-text
DOCUMENT NUMBER: 145:28029
TITLE: Preparation of oxaazabenzocycloheptyl malonamides as γ-secretase inhibitors.
INVENTOR(S): Flohr, Alexander; Jakob-Roetne, Roland; Wostl, Wolfgang
PATENT ASSIGNEE(S): Hoffmann-La Roche Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 58 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006122168	A1	20060608	US 2005-289176	20051130
US 7211573	B2	20070501		
WO 2006061136	A2	20060615	WO 2005-EP12834	20051201
WO 2006061136	A3	20060803		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: EP 2004-106395 A 20041208
EP 2005-100816 A 20050207

OTHER SOURCE(S): MARPAT 145:28029
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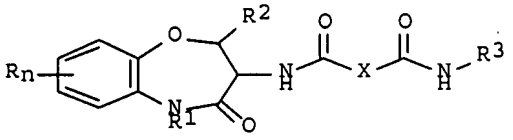


I

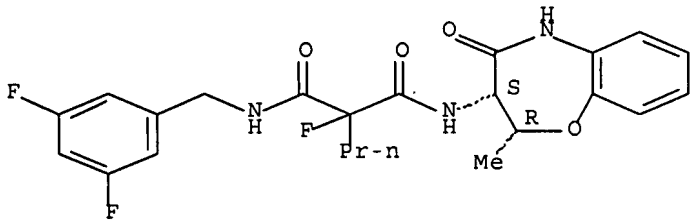
AB Title compds. [I; R = halo, (halo)alkyl; R1 = R, hydroxylalkyl, alkenyl, (halo)benzyl, cycloalkyl(alkyl), etc.; R2 = H, (halo- or hydroxy-substituted) alkyl, benzyl, cycloalkyl; R3 = (halo)alkyl, (halo)benzyl, cycloalkyl(alkyl), pyridyl(alkyl); X = CR4R4', CR4R4'O; R4, R4' = H, halo, alkyl, alkoxy, OH, etc.; n = 0-2], were prepared Thus, N-[(6R,7S)-2-fluoro-9-(2-hydroxyethyl)-6-methyl-8-oxo-6,7,8,9-tetrahydro-5- oxa-9-azabenzocyclohepten-7-yl]-2-(R or S)-

hydroxy-2-methyl-N-(2,2,3,3,3- pentafluoropropyl)malonamide entity A (multistep preparation given) inhibited γ-secretase with IC50 = 7 nM.

IT ***889457-84-5P 889457-85-6P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of oxaazabenzocycloheptyl malonamides as γ-secretase inhibitors)

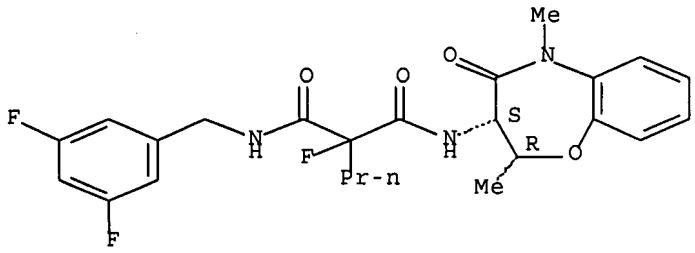
RN 889457-84-5 CAPLUS
CN Propanediamide, N-[(3,5-difluorophenyl)methyl]-2-fluoro-2-propyl-N'-[(2R,3S)-2,3,4,5-tetrahydro-2-methyl-4-oxo-1,5-benzoxazepin-3-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 889457-85-6 CAPLUS
CN Propanediamide, N-[(3,5-difluorophenyl)methyl]-2-fluoro-2-propyl-N'-[(2R,3S)-2,3,4,5-tetrahydro-2,5-dimethyl-4-oxo-1,5-benzoxazepin-3-yl]- (9CI) (CA INDEX NAME)

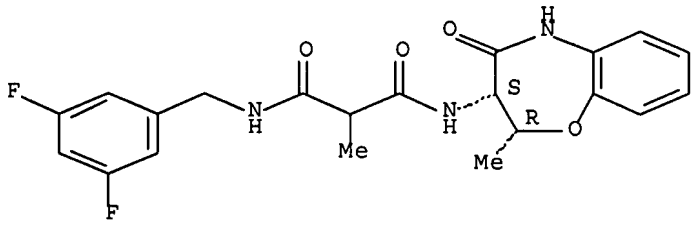
Absolute stereochemistry.



IT ***889458-03-1P 889458-05-3P 889458-14-4P 889458-15-5P 889458-42-8P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of oxaazabenzocycloheptyl malonamides as γ-secretase inhibitors)

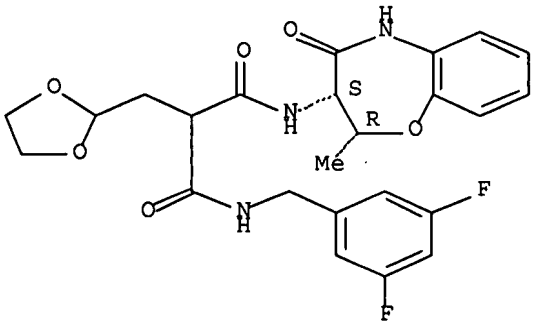
RN 889458-03-1 CAPLUS
CN Propanediamide, N-[(3,5-difluorophenyl)methyl]-2-methyl-N'-[(2R,3S)-2,3,4,5-tetrahydro-2-methyl-4-oxo-1,5-benzoxazepin-3-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



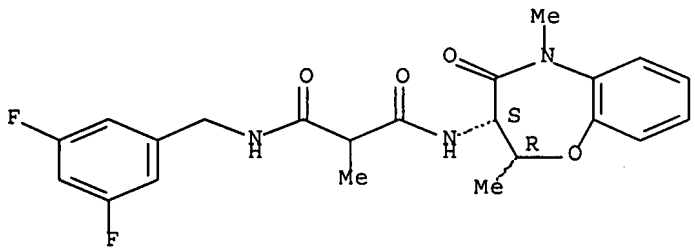
RN 889458-05-3 CAPLUS
CN Propanediamide, N-[(3,5-difluorophenyl)methyl]-2-(1,3-dioxolan-2-ylmethyl)-N'-[(2R,3S)-2,3,4,5-tetrahydro-2-methyl-4-oxo-1,5-benzoxazepin-3-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



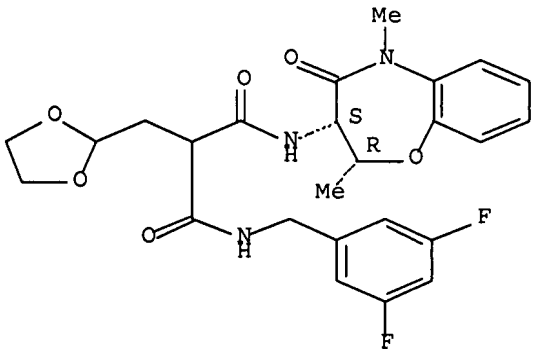
RN 889458-14-4 CAPLUS
CN Propanediamide, N-[(3,5-difluorophenyl)methyl]-2-methyl-N'-[(2R,3S)-2,3,4,5-tetrahydro-2,5-dimethyl-4-oxo-1,5-benzoxazepin-3-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



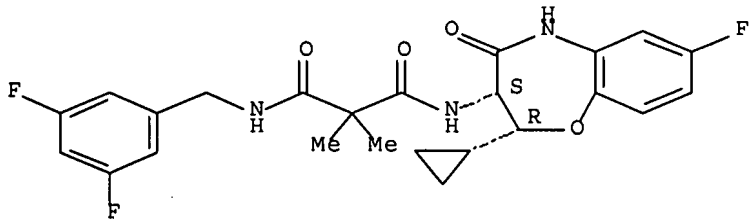
RN 889458-15-5 CAPLUS
CN Propanediamide, N-[(3,5-difluorophenyl)methyl]-2-(1,3-dioxolan-2-ylmethyl)-N'-[(2R,3S)-2,3,4,5-tetrahydro-2,5-dimethyl-4-oxo-1,5-benzoxazepin-3-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 889458-42-8 CAPLUS
CN Propanediamide, N-[(2R,3S)-2-cyclopropyl-7-fluoro-2,3,4,5-tetrahydro-4-oxo-1,5-benzoxazepin-3-yl]-N'-[(3,5-difluorophenyl)methyl]-2,2-dimethyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L53 ANSWER 3 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1314177 CAPLUS Full-text
DOCUMENT NUMBER: 144:51616
TITLE: Preparation of diazepinediones as ligands of melanocortin 1 and/or 4 receptors
INVENTOR(S): Szewczyk, Jerzy Ryszard; Speake, Jason Daniel; Sammond, Douglas Mccord; Sherrill, Ronald George
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 92 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005118573	A1	20051215	WO 2005-US18773	20050527

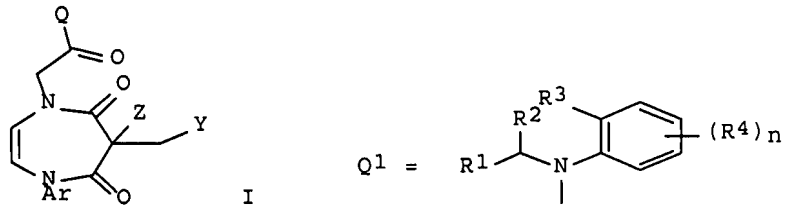
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,

SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2004-575644P P 20040528

OTHER SOURCE(S): MARPAT 144:51616

GI



AB Title compds. [I; Ar = (substituted) aryl, heteroaryl; Y = specified indazolyl, benzimidazolyl, oxobenzimidazolyl; Z = H, alkoxy; Q = Q1; R1, R2, R4 = H, OH, haloalkyl, alkoxy, haloalkoxy, amino; n = 0-2; R3 = H; R2R3 = atoms to form 6-7 membered ring], were prepared Thus, 2-[2,4-dioxo-3-(1H-indazol-3-ylmethylene)-5-phenyl-2,3,4,5-tetrahydro-1H- 1,5-diazepin-1-yl]-N-(4-chlorophenyl)-N-isopropylacetamide hydrochloride (multistep preparation given) showed MC4R agonist activity with pEC50 = 7.37.

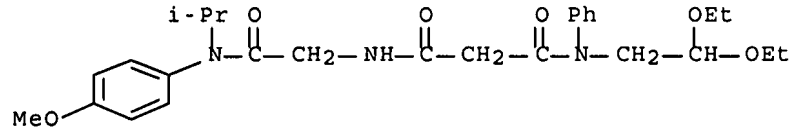
IT ***179083-73-9P 179083-74-0P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of diazepinediones as ligands of melanocortin-1 and/or 4 receptors)

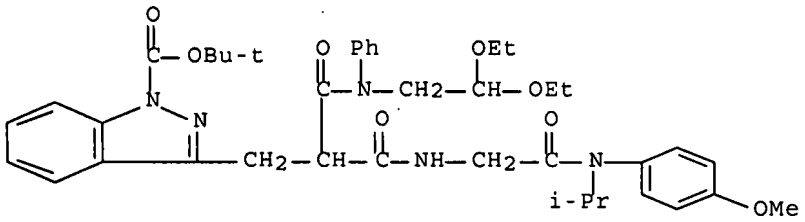
RN 179083-73-9 CAPLUS

CN Glycinamide, N-(2,2-diethoxyethyl)-3-oxo-N-phenyl-β-alanyl-N-(4-methoxyphenyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 179083-74-0 CAPLUS

CN Glycinamide, N-(2,2-diethoxyethyl)-2-[[1-[(1,1-dimethylethoxy)carbonyl]-1H-indazol-3-yl]methyl]-3-oxo-N-phenyl-β-alanyl-N-(4-methoxyphenyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

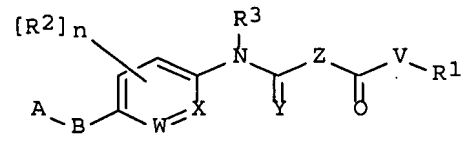
L53 ANSWER 4 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1176889 CAPLUS Full-text
DOCUMENT NUMBER: 143:440434
TITLE: Preparation of monocyclic heterocycles as kinase inhibitors, particularly Met kinase, for treating cancer
INVENTOR(S): Borzilleri, Robert M.; Cornelius, Lyndon A. M.; Schmidt, Robert J.; Schroeder, Gretchen M.; Kim, Kyoung S.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 128 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005245530	A1	20051103	US 2005-111144	20050421
AU 2005249382	A1	20051215	AU 2005-249382	20050422
CA 2563831	A1	20051215	CA 2005-2563831	20050422
WO 2005117867	A2	20051215	WO 2005-US14120	20050422
WO 2005117867	A3	20060330		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1737451	A2	20070103	EP 2005-779444	20050422
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR, LV, MK, YU				
NO 2006005148	A	20061108	NO 2006-5148	20061108

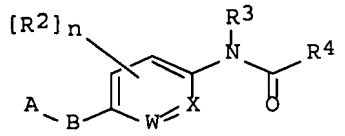
PRIORITY APPLN. INFO.:		
US 2004-564842P	P	20040423
US 2004-639178P	P	20041223
US 2005-111144	A	20050421
WO 2005-US14120	W	20050422

OTHER SOURCE(S): MARPAT 143:440434

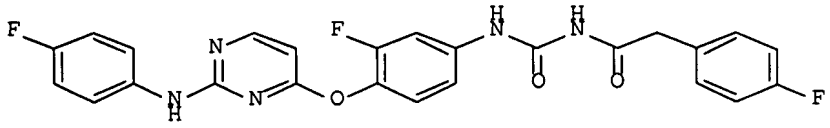
GI



I



II



III

AB The invention is related to compds. of formula I and II [wherein R1 = H, (un)substituted alk(en/yn)yl, hetero/aryl, etc.; each R2 = independently H, halo, CN, NO2, alkyl, etc.; B = O, S, SO, SO2, NH, etc.; V = NH and derivs., (CH2)p and derivs. with proviso; p = 0-4; W, X = independently C, N; Z = CH2 and derivs.; (CH2)q-NH and derivs.; q = 0-2; R3 = H, (un)substituted heterocyclyl, alk(en/yn)yl, cycloalkyl, hetero/aryl, etc.,; R4 = (un)substituted hetero/aryl, heterocycloalkyl with provisos; A = (un)substituted pyridin-4-yl, pyrimidin-4-yl, pyridazin-4-yl, etc.] their enantiomers, diastereomers, hydrates, solvates, and pharmaceutically acceptable salts, as protein kinase, particularly Met kinase, inhibitors and methods for using them for the treatment of cancer. E.g., a 4 step synthesis of pyrimidine II, starting from 2,4-dichloropyrimidine and N-(3-fluoro-4-hydroxyphenyl)acetamide, was given. Preferred compds. I inhibited Met kinase with IC50 values between 0.01 and 100 μM.

IT *868736-02-1P*

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

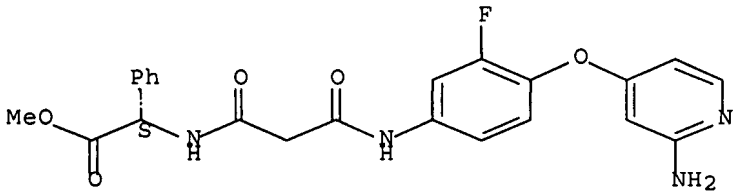
(drug candidate; preparation of monocyclic heterocycles as kinase inhibitors

for treating cancer)

RN 868736-02-1 CAPLUS

CN Benzeneacetic acid, α-[[3-[[4-[(2-amino-4-pyridinyl)oxy]-3-fluorophenyl]amino]-1,3-dioxopropyl]amino]-, methyl ester, monohydrochloride, (αS)- (9CI) (CA INDEX NAME)

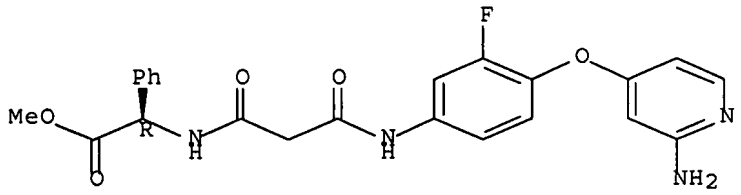
Absolute stereochemistry.



● HCl

IT *868736-03-2P*
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of monocyclic heterocycles as kinase inhibitors
for treating cancer)
RN 868736-03-2 CAPLUS
CN Benzeneacetic acid, α-[[3-[[4-[(2-amino-4-pyridinyl)oxy]-3-fluorophenyl]amino]-1,3-dioxopropyl]amino]-, methyl ester, monohydrochloride, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

L53 ANSWER 5 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:323777 CAPLUS Full-text
DOCUMENT NUMBER: 142:378922
TITLE: Method for decreasing sebum production using malonamide acyl CoA cholesterol acyl transferase inhibitors
INVENTOR(S): Kostlan, Catherine R.; Raheja, Raj Neil; Tugnait, Meera; Wade, Kimberly
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 17 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 2005079144	A1	20050414	US 2004-958306	20041005
AU 2004280134	A1	20050421	AU 2004-280134	20040927
CA 2541814	A1	20050421	CA 2004-2541814	20040927
WO 2005034931	A1	20050421	WO 2004-IB3156	20040927

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1673077	A1	20060628	EP 2004-769499	20040927

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

CN 1863521	A	20061115	CN 2004-80029467	20040927
BR 2004015136	A	20061128	BR 2004-15136	20040927
JP 2007508291	T	20070405	JP 2006-530738	20040927
NO 2006001277	A	20060629	NO 2006-1277	20060321
PRIORITY APPLN. INFO.:			US 2003-509984P P	20031009
			WO 2004-IB3156 W	20040927

OTHER SOURCE(S): MARPAT 142:378922

AB The present invention is directed to the topical application of the malonamide acyl CoA cholesterol acyl transferase (ACAT) inhibitors. Other aspects of the invention are directed to topical formulations of these diamides, their use to treat sebaceous gland disorders and their use to alleviate oily skin. Efficacy of a series of ACAT inhibitors in decreasing sebum production in hamster ear sebaceous glands is shown.

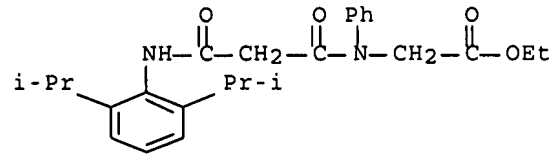
IT ***137379-32-9***

RL: COS (Cosmetic use); PAC (Pharmacological activity); BIOL (Biological study); USES (Uses)

(method for decreasing sebum production using malonamide acyl CoA cholesterol acyl transferase inhibitors)

RN 137379-32-9 CAPLUS

CN Glycine, N-[3-[[2,6-bis(1-methylethyl)phenyl]amino]-1,3-dioxopropyl]-N-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



L53 ANSWER 6 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:652532 CAPLUS Full-text

DOCUMENT NUMBER: 141:172870

TITLE: Conjugates of haptens and β-lactam derivatives for quantifying haptens in solution and device for implementation thereof

INVENTOR(S): Kohl, Michel; Renotte, Roger; Sarlet, Guy; Lejeune,

Robert; Granier, Benoit
PATENT ASSIGNEE(S): Belg.
SOURCE: U.S. Pat. Appl. Publ., 33 pp., Cont.-in-part of U.S. Ser. No. 171,819.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

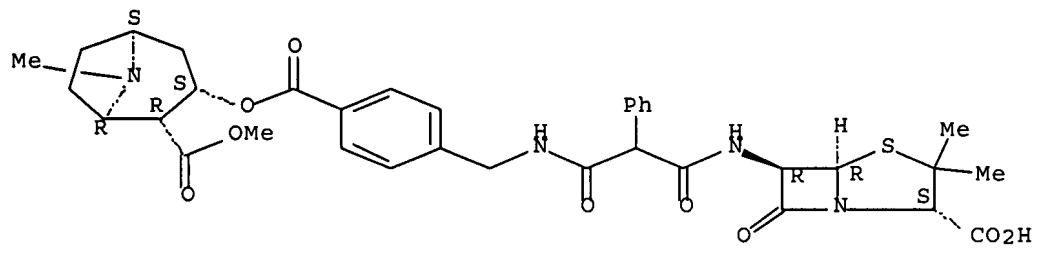
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004157262	A1	20040812	US 2001-915211	20010725
BE 1010184	A3	19980203	BE 1996-384	19960430
US 6436649	B1	20020820	US 1999-171819	19990611
PRIORITY APPLN. INFO.:			BE 1996-384 A	19960430
			US 1999-171819 A2	19990611
			WO 1997-BE52 W	19970430

AB The present invention is related to a conjugate of a hapten to a natural or synthetic β-lactam derivative, comprising at least a side chain, wherein the side chain of the β-lactam derivative is at least partially constitutive of the conjugating arm. The invention relates also to a method for the immunoassay of the hapten involving said β-lactam derivative-hapten conjugate as an inhibitor for a lactamase or a penicillin detector capable of specific recognition of the β-lactamic moiety of said conjugate. The hapten is a steroid, drug of abuse and medicine e.g. nandrolone, testosterone, progesterone, estradiol and cocaine; and the β-lactam derivative is a penicillin derivative or cephalosporin derivative e.g. carbenicillin, oxacillin, cefuroxime, cefotaxime, methicillin, benzylpenicillin and phenoxymethylpenicillin.

IT *198830-23-8P*
RL: ARU (Analytical role, unclassified); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(conjugates of haptens and β-lactam derivs. for quantifying haptens in solution and device for implementation thereof)

RN 198830-23-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[[4-[[[3-[[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]amino]-1,3-dioxo-2-phenylpropyl]amino]methyl]benzoyl]oxy]-8-methyl-, 2-methyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 7 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:648538 CAPLUS Full-text
DOCUMENT NUMBER: 141:191072
TITLE: Preparation and use of chemically-modified metabolites of regulatory peptides
INVENTOR(S): Peri, Krishna; Habi, Abdelkrim; Gravel, Denis
PATENT ASSIGNEE(S): Theratechnologies Inc., Can.
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004067548	A2	20040812	WO 2004-CA131	20040130
WO 2004067548	A3	20041209		
WO 2004067548	B1	20050217		
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI				
US 2005059605	A1	20050317	US 2004-768974	20040130
PRIORITY APPLN. INFO.:			US 2003-443860P P	20030131
OTHER SOURCE(S):		MARPAT 141:191072		

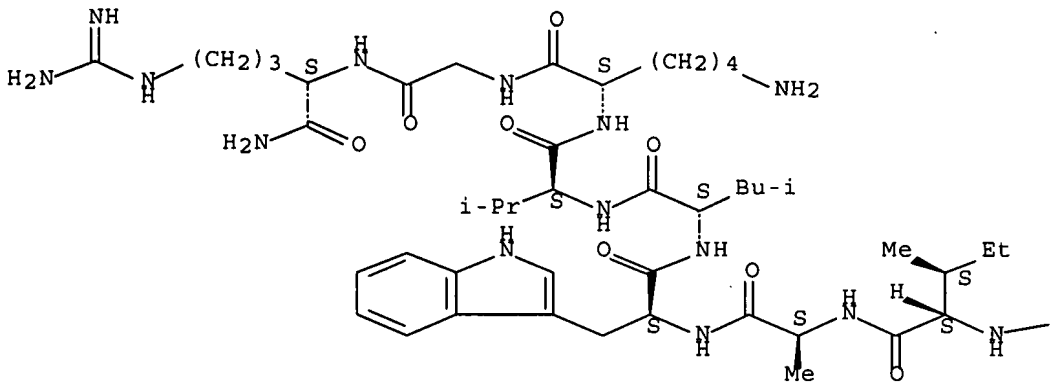
AB The invention relates to peptides B-A-CO-P or their pharmaceutically-acceptable salts, where P is a dipeptidyl-peptidase (DPPIV) peptide metabolite of regulatory peptides obtained by cleavage of the two N-terminal amino acids, A is (hetero)alk(en)(yn)ylene or Ph and B is (un)substituted (hetero)aryl or cycloalkyl. More specifically, the invention relates to conferring biol. activity to metabolites of regulatory peptides by the covalent coupling of small mols. Thus, 3-(4-methoxyphenethylamino)-3-oxopropanoyl-GLP-1 (9-36) was prepared by solid-phase peptide chemical and N-acylation and shown to produce a more significant hypoglycemic response in mice compared to native GLP-1.

IT ***736176-31-1P 736176-32-2P 736176-38-8P 736176-39-9P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and use of chemical-modified metabolites of regulatory peptides)

RN 736176-31-1 CAPLUS
CN L-Argininamide, 3-oxo-N-(2-phenylethyl)-β-alanyl-L-α-glutamylglycyl-L-threonyl-L-phenylalanyl-L-threonyl-L-seryl-L-α-aspartyl-L-valyl-L-seryl-L-seryl-L-tyrosyl-L-leucyl-L-α-glutamylglycyl-L-glutaminyl-L-alanyl-L-alanyl-L-lysyl-L-α-glutamyl-L-phenylalanyl-L-isoleucyl-L-alanyl-L-tryptophyl-L-leucyl-L-valyl-L-lysylglycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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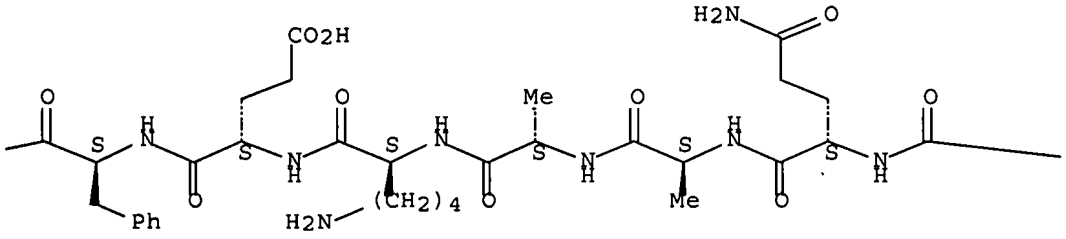

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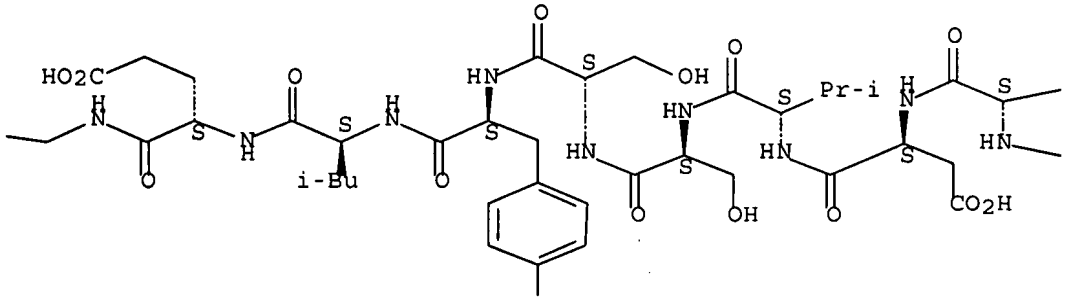

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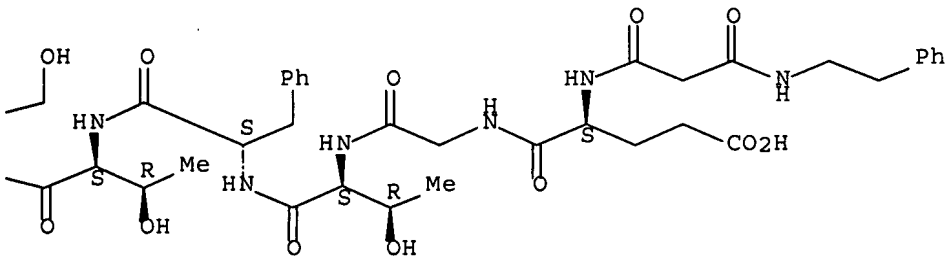


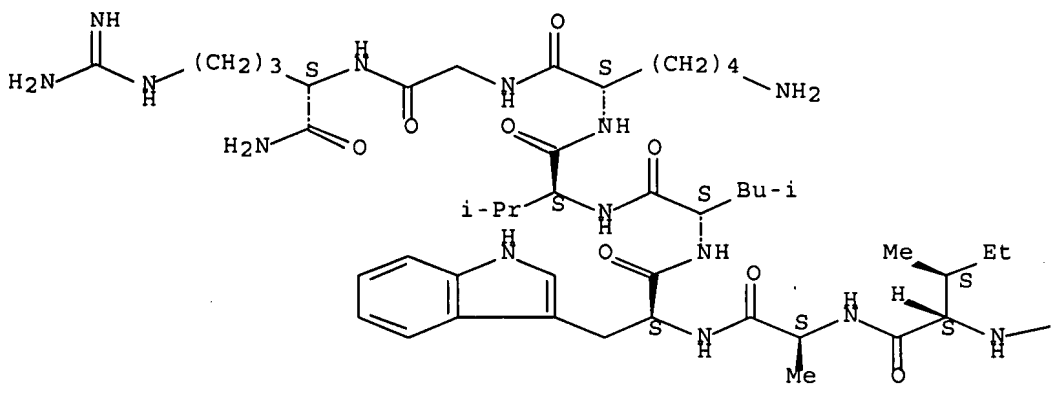
PAGE 2-C

RN 736176-32-2 CAPLUS

CN L-Argininamide, N-[2-(4-methoxyphenyl)ethyl]-3-oxo-β-alanyl-L-α-glutamylglycyl-L-threonyl-L-phenylalanyl-L-threonyl-L-seryl-L-α-aspartyl-L-valyl-L-seryl-L-seryl-L-tyrosyl-L-leucyl-L-α-glutamylglycyl-L-glutaminyl-L-alanyl-L-alanyl-L-lysyl-L-α-glutamyl-L-phenylalanyl-L-isoleucyl-L-alanyl-L-tryptophyl-L-leucyl-L-valyl-L-lysylglycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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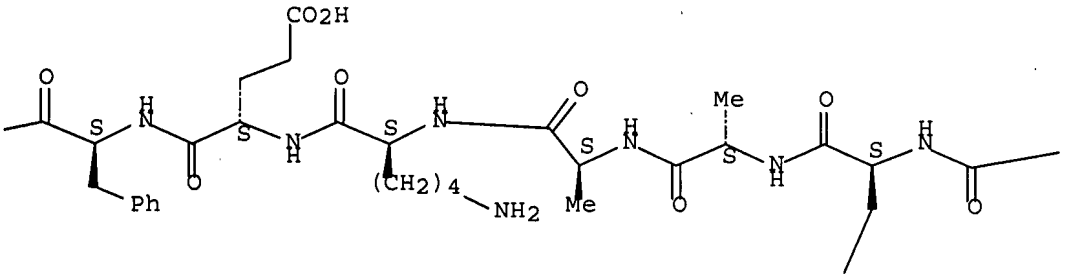

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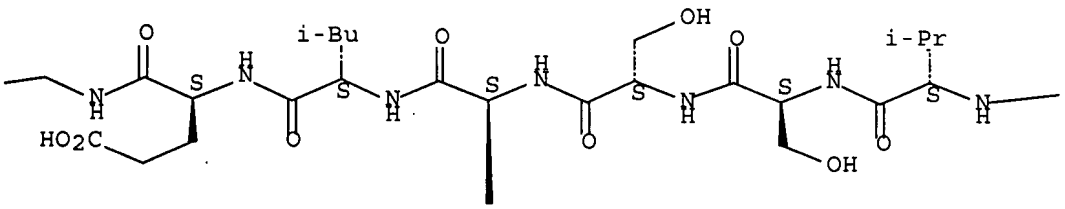

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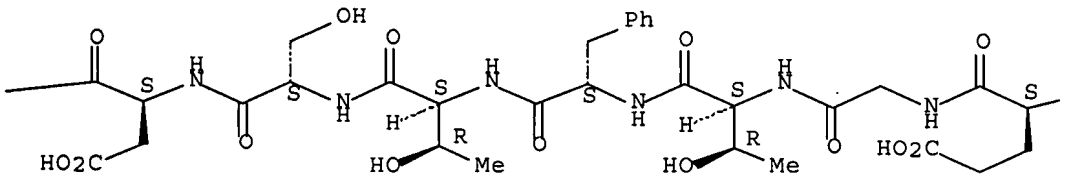

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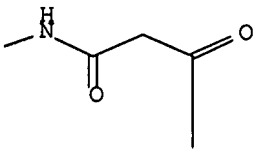

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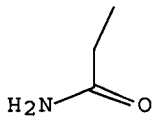

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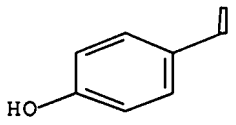

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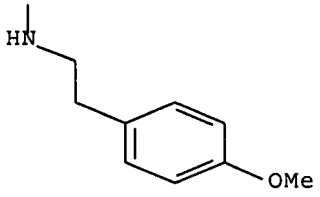
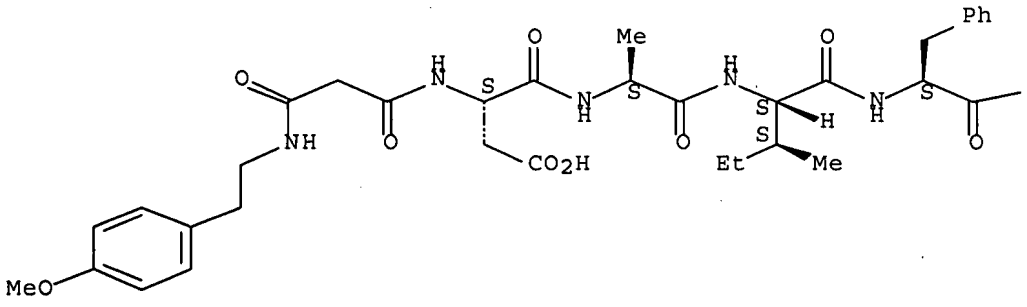


RN 736176-38-8 CAPLUS

CN L-Argininamide, N-[2-(4-methoxyphenyl)ethyl]-3-oxo-β-alanyl-L-α-aspartyl-L-alanyl-L-isoleucyl-L-phenylalanyl-L-threonyl-L-asparaginyl-L-seryl-L-tyrosyl-L-arginyl-L-lysyl-L-valyl-L-leucylglycyl-L-glutaminyl-L-leucyl-L-seryl-L-alanyl-L-arginyl-L-lysyl-L-leucyl-L-leucyl-L-glutaminyl-L-α-aspartyl-L-isoleucyl-L-methionyl-L-seryl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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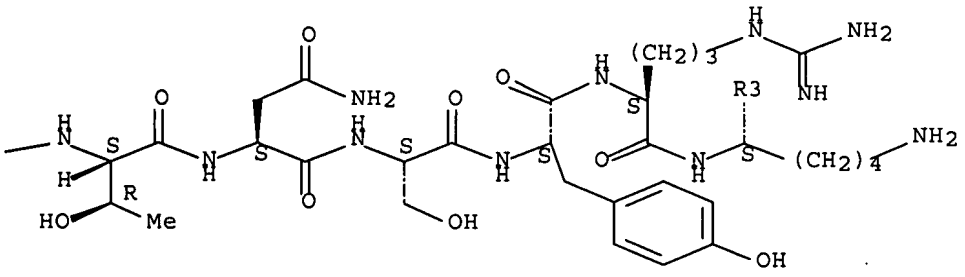

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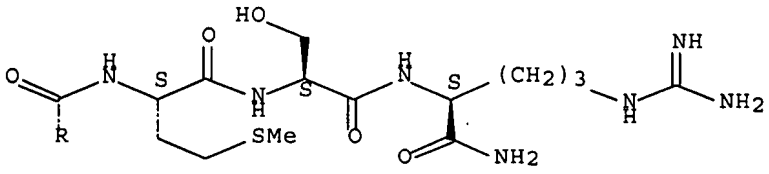

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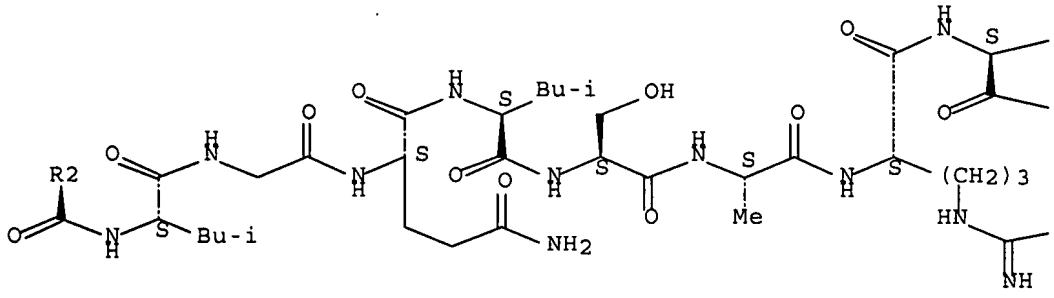
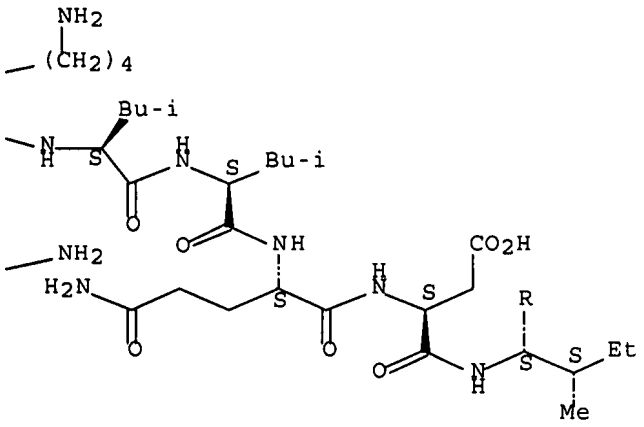


PAGE 3-B



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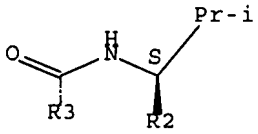
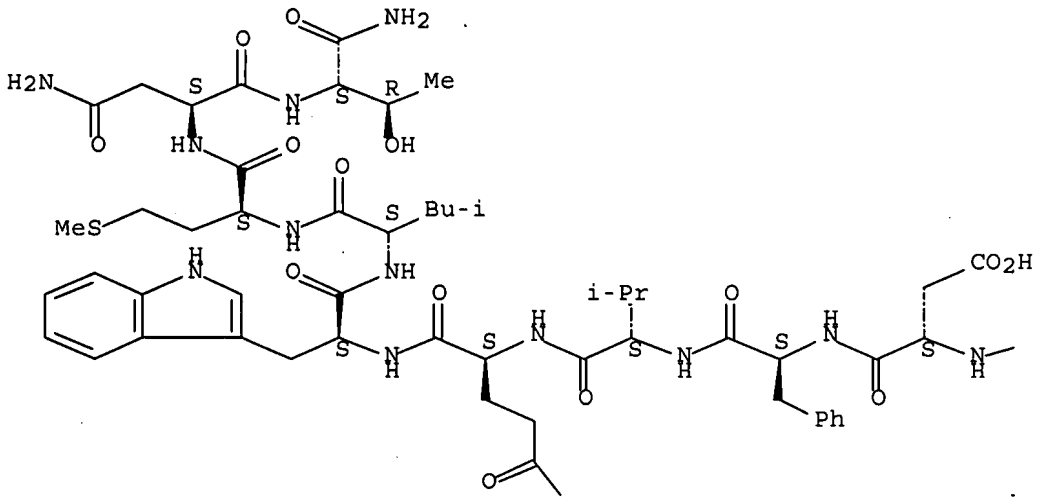


RN 736176-39-9 CAPLUS

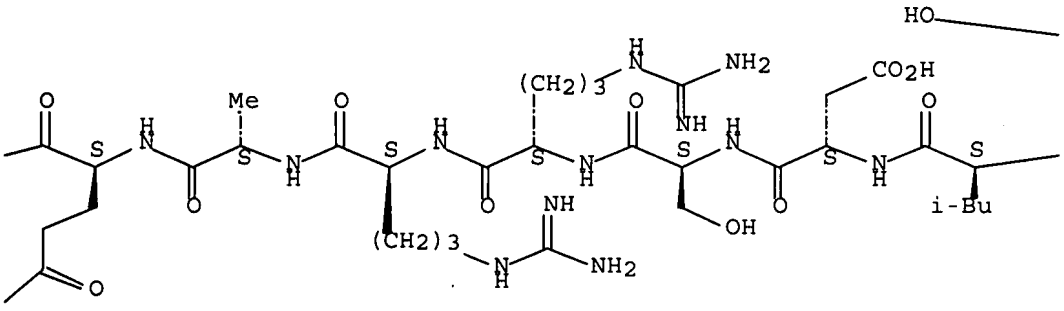
CN L-Threoninamide, N-[2-(4-methoxyphenyl)ethyl]-3-oxo-β-alanyl-L-glutaminylglycyl-L-threonyl-L-phenylalanyl-L-threonyl-L-seryl-L-α-aspartyl-L-tyrosyl-L-seryl-L-lysyl-L-tyrosyl-L-leucyl-L-α-aspartyl-L-seryl-L-arginyl-L-arginyl-L-alanyl-L-glutaminyl-L-α-aspartyl-L-phenylalanyl-L-valyl-L-glutaminyl-L-tryptophyl-L-leucyl-L-methionyl-L-asparaginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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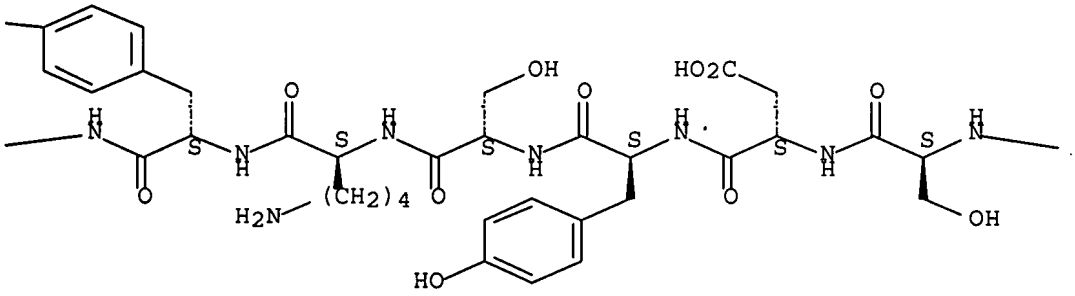

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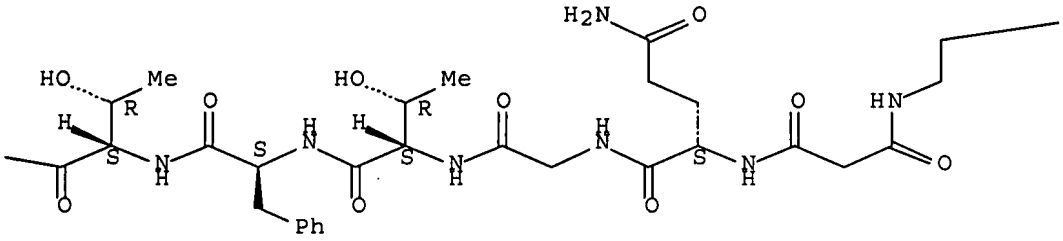

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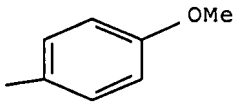

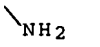

L53 ANSWER 8 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:946095 CAPLUS Full-text
DOCUMENT NUMBER: 138:24322
TITLE: Preparation of malonamides as cathepsin inhibitors
INVENTOR(S): Patterson, John W.; Zipfel, Sheila
PATENT ASSIGNEE(S): Celera, USA
SOURCE: PCT Int. Appl., 67 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002098406	A1	20021212	WO 2002-US17922		20020604
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2449021	A1	20021212	CA 2002-2449021		20020604
AU 2002312357	A1	20021216	AU 2002-312357		20020604
EP 1399146	A1	20040324	EP 2002-739721		20020604
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BR 2002010172	A	20040622	BR 2002-10172		20020604
CN 1512880	A	20040714	CN 2002-811289		20020604
JP 2005500275	T	20050106	JP 2003-501445		20020604
NZ 529903	A	20050930	NZ 2002-529903		20020604
US 2004147503	A1	20040729	US 2003-478632		20031124
NO 2003005365	A	20040220	NO 2003-5365		20031202
ZA 2003009371	A	20050527	ZA 2003-9371		20031202
IN 2003DN02092	A	20060120	IN 2003-DN2092		20031204
PRIORITY APPLN. INFO.:			US 2001-295744P	P	20010604
			WO 2002-US17922	W	20020604

OTHER SOURCE(S): MARPAT 138:24322
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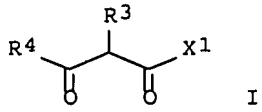

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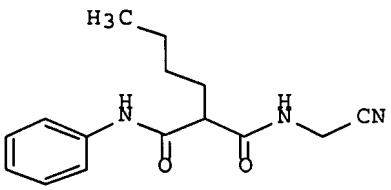


II

AB The title malonamides I [wherein X1 = substituted amino; R3 = (un)substituted alkyl; R4 = (un)substituted amino; with provisos; and the N-oxide derivs., prodrugs, protected derivs., isomers, mixts. of isomers, pharmaceutically acceptable salts, and solvates thereof] were prepared as selective cathepsin S inhibitors. For example, a solution of aniline in CH2Cl2 was treated with Me malonyl chloride in the presence of Et3N, followed by reaction with 1-iodobutane in N-methylpyrrolidinone in the presence of LiOH to give Me 2-phenylcarbamoylhexanoate. The above compound was treated with NaOH in MeOH, followed by the addition of 1 N aqueous HCl solution to afford 2-phenylcarbamoylhexanoic acid (74%). The hexanoic acid in DMF was treated with PyBOP, aminoacetonitrile bisulfate, and Et3N to provide 2-butyl-N-cyanomethyl-N'-phenylmalonamide (II) (57%). I showed inhibition consts. against cathepsin S in the range of 10-10 M to 10-7 M. Pharmaceutical formulations containing a compound of formula I were also presented.

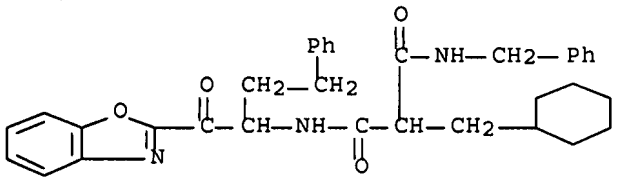
IT ***477860-82-5P 477861-17-9P***

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(cathepsin inhibitor; preparation of malonamides via condensation reactions of malonic acids with amines as cathepsin inhibitors)

RN 477860-82-5 CAPLUS

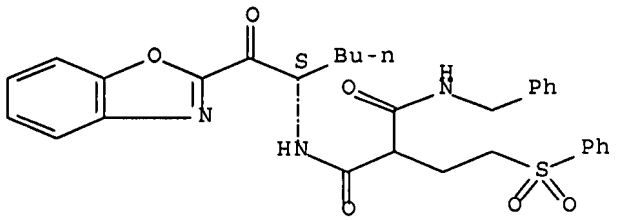
CN Propanediamide, N-[1-(2-benzoxazolylcarbonyl)-3-phenylpropyl]-2-(cyclohexylmethyl)-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 477861-17-9 CAPLUS

CN Propanediamide, N-[(1S)-1-(2-benzoxazolylcarbonyl)pentyl]-N'-(phenylmethyl)-2-[2-(phenylsulfonyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 9 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:631914 CAPLUS Full-text
DOCUMENT NUMBER: 135:195426
TITLE: Preparation of malonic acid amide derivatives as inhibitors of blood clotting factor Xa
INVENTOR(S): Al-Obeidi, Fahad; Walser, Armin; Wildgoose, Peter
PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany
SOURCE: Eur. Pat. Appl., 69 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 1127884	A1	20010829	EP 2000-104041		20000226
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
BR 2001008694	A	20021210	BR 2001-8694		20010121
CA 2400871	A1	20010830	CA 2001-2400871		20010221
WO 2001062735	A1	20010830	WO 2001-EP1928		20010221
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
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EP 1265867	B1	20051228			
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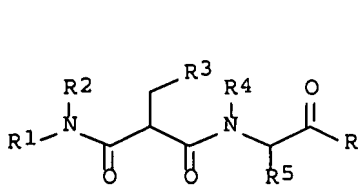
HU 200300080	A2	20030628	HU 2003-80		20010221
JP 2003524001	T	20030812	JP 2001-562517		20010221
NZ 520982	A	20040528	NZ 2001-520982		20010221
AT 314350	T	20060115	AT 2001-907546		20010221
ES 2254370	T3	20060616	ES 2001-1907546		20010221
US 2002022596	A1	20020221	US 2001-790641		20010223
US 6794365	B2	20040921			
ZA 2002006581	A	20030728	ZA 2002-6581		20020816
NO 2002004040	A	20020924	NO 2002-4040		20020823
PRIORITY APPLN. INFO.:			EP 2000-104041	A	20000226
			WO 2001-EP1928	W	20010221

OTHER SOURCE(S): MARPAT 135:195426
GI



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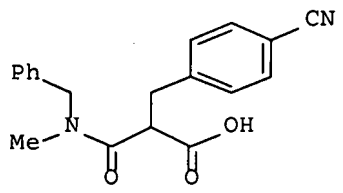

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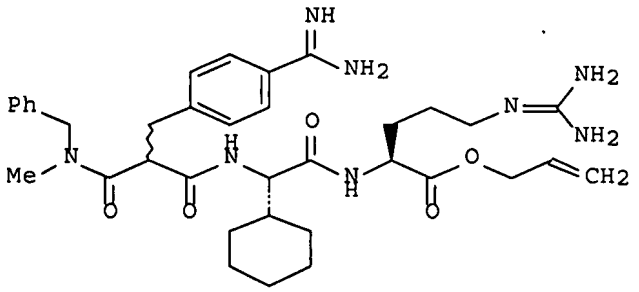


III

AB Title compds. I [R1 = H, alk(en)yl, aryl(alkyl); R2 = H,alkyl; R3 = aryl; R4 = H, alkyl, etc.; R5 = (cyclo)alkyl, cycloalkyl-alkyl, aryl(alkyl), etc.; R6 = NH2, OH or substituted derivs.] are prepared Examples included 3 synthetic procedures (including a general solid phase method), over 100 compds. prepared and 8 bioassays (data provided for 1 of the bioassays). For instance, benzyl Me amine was treated with bis(trimethylsilyl)acetamide (DCM, reflux, 3 h) followed by addition of 4-[(2,2-dimethyl-4,6-dioxo-1,3-dioxan-5-yl)methyl]benzonitrile (DCM, reflux, 3 h) to give II. II was coupled to (αS)-amino-cyclohexane- acetic acid Me ester (iPr2EtN, HODhbt, DCC, DMF, 10°C) and the resulting amide-nitrile reacted with excess hydroxylamine (EtOH, reflux, 4 h) to give the corresponding N-hydroxy carbamimidoyl derivative This intermediate was deoxygenated (Pd-H2/C), hydrolyzed (HClaq, CH3CN, 4 days @ room temperature) and coupled with (S)-2-amino-5-guanidinopentanoic acid allyl ester (DMF, collidine, HATU) to give III. Isomers of III were separated by chromatog. (MPLC, RP18) and isolated as the trifluoroacetic acid salts. An isomer of III had Ki = 0.0010 μM for factor Xa. The invention also provides methods for the treatment/prevention of (e.g.) thromboembolic diseases.

IT ***356543-22-1P 356543-24-3P 356543-26-5P***
356543-28-7P 356543-36-7P 356543-38-9P
356543-46-9P 356543-51-6P 356543-57-2P
356543-69-6P 356543-75-4P 356543-83-4P
356543-91-4P 356543-99-2P 356544-07-5P
356544-15-5P 356544-24-6P 356544-32-6P
356544-36-0P 356544-52-0P 356544-62-2P
356544-68-8P 356544-74-6P 356544-80-4P
356545-29-4P 356545-35-2P 356545-43-2P
356545-45-4P 356545-47-6P 356545-53-4P
356545-55-6P 356545-60-3P 356545-66-9P
356545-67-0P 356545-69-2P 356545-71-6P
356545-73-8P 356545-75-0P 356545-77-2P
356545-79-4P 356545-81-8P 356545-83-0P
356545-85-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug; preparation of malonic acid amide derivs. as inhibitors of blood clotting factor Xa)

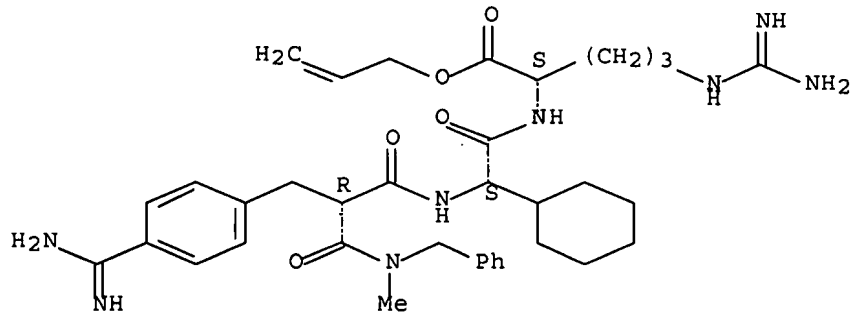
RN 356543-22-1 CAPLUS

CN L-Arginine, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, 2-propenyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

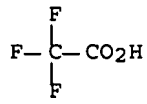
CRN 356543-21-0
CMF C36 H50 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

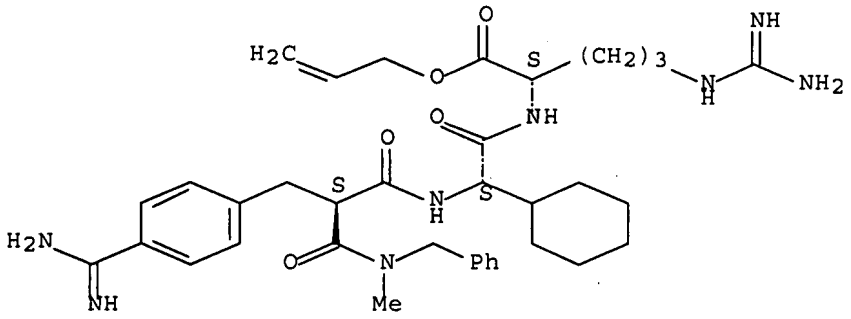


RN 356543-24-3 CAPLUS
CN L-Arginine, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, 2-propenyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

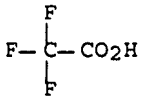
CRN 356543-23-2
CMF C36 H50 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

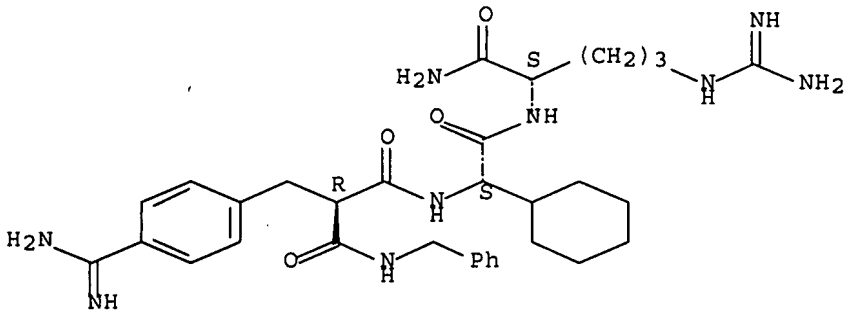


RN 356543-26-5 CAPLUS
CN L-Argininamide, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

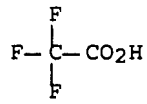
CRN 356543-25-4
CMF C32 H45 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

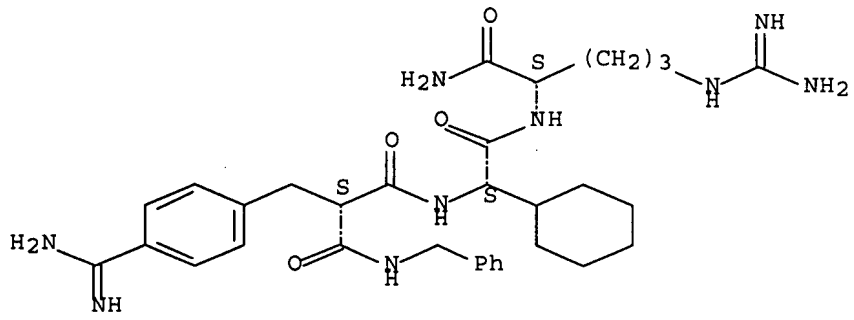


RN 356543-28-7 CAPLUS
CN L-Argininamide, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

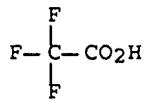
CRN 356543-27-6
CMF C32 H45 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

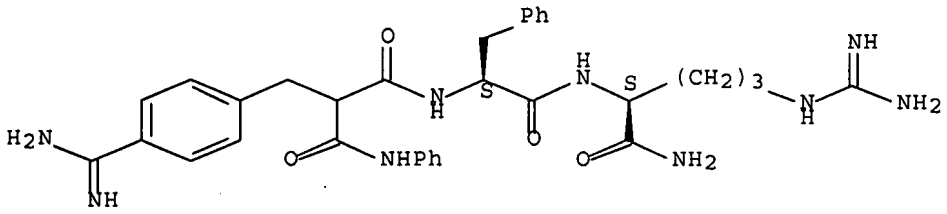


RN 356543-36-7 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-L-phenylalanyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

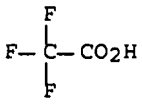
CRN 356543-35-6
CMF C32 H39 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

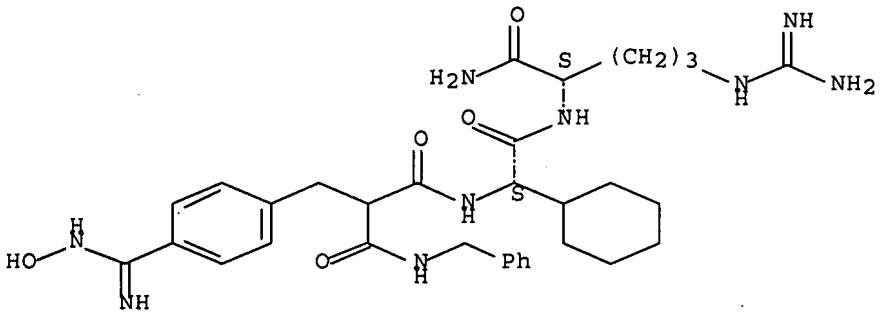


RN 356543-38-9 CAPLUS
CN L-Argininamide, 2-[[4-[(hydroxyamino)iminomethyl]phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

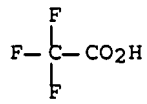
CRN 356543-37-8
CMF C32 H45 N9 O5

Absolute stereochemistry.



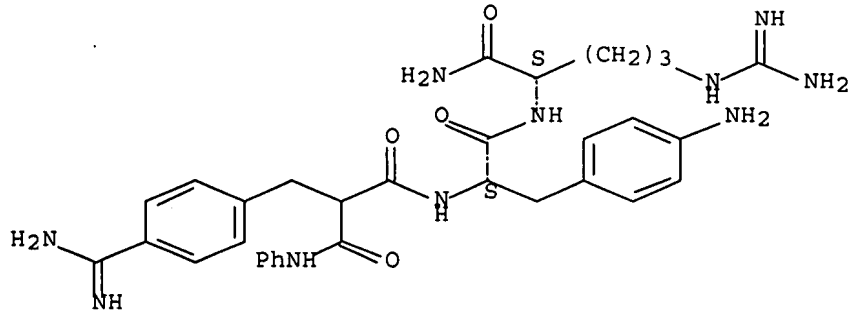
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 356543-46-9 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-4-amino-L-phenylalanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

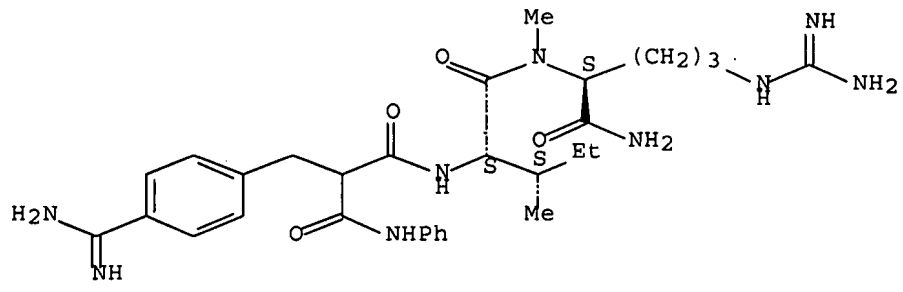


RN 356543-51-6 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-L-isoleucyl-N2-methyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

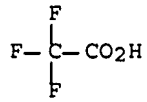
CRN 356543-50-5
CMF C30 H43 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

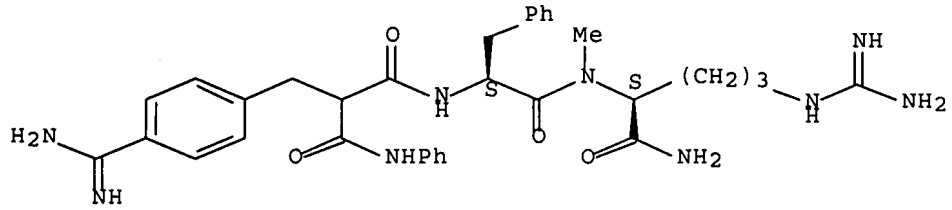


RN 356543-57-2 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-L-phenylalanyl-N2-methyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

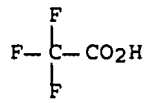
CRN 356543-56-1
CMF C33 H41 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

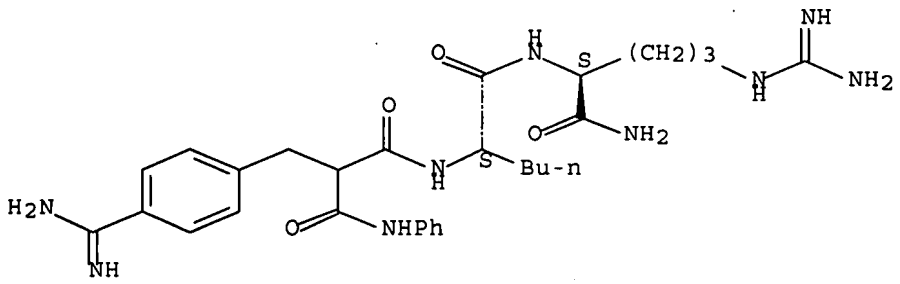


RN 356543-69-6 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-L-norleucyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

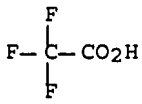
CRN 356543-68-5
CMF C29 H41 N9 O4

Absolute stereochemistry.



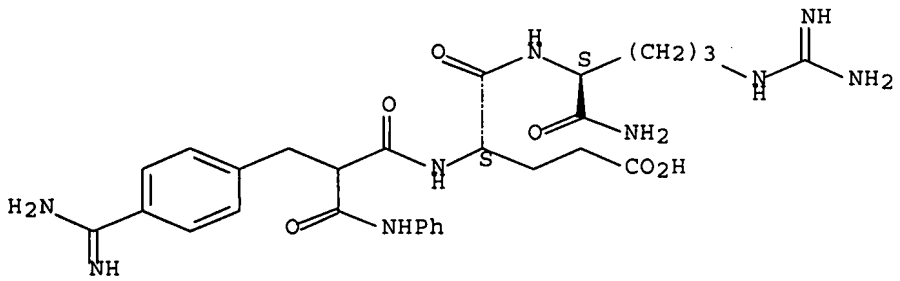
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 356543-75-4 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-L-α-glutamyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

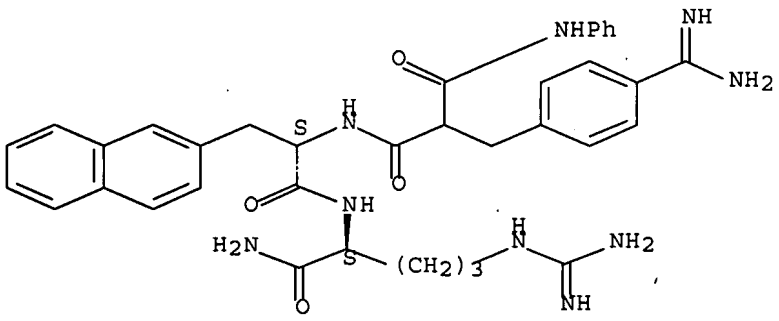


RN 356543-83-4 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-3-(2-naphthalenyl)-L-alanyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

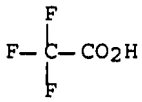
CRN 356543-82-3
CMF C36 H41 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

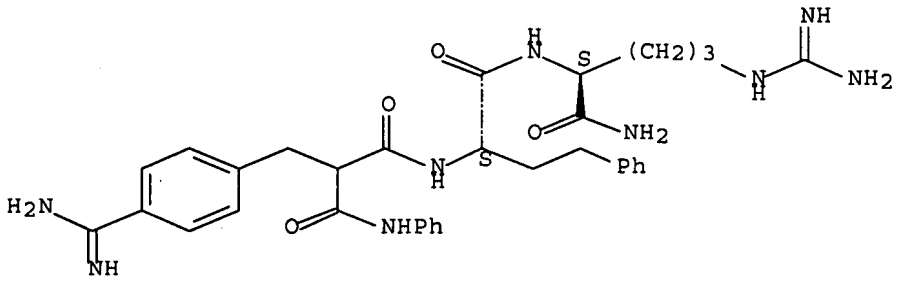


RN 356543-91-4 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-(αS)-α-aminobenzenebutanoyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

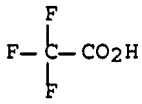
CRN 356543-90-3
CMF C33 H41 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

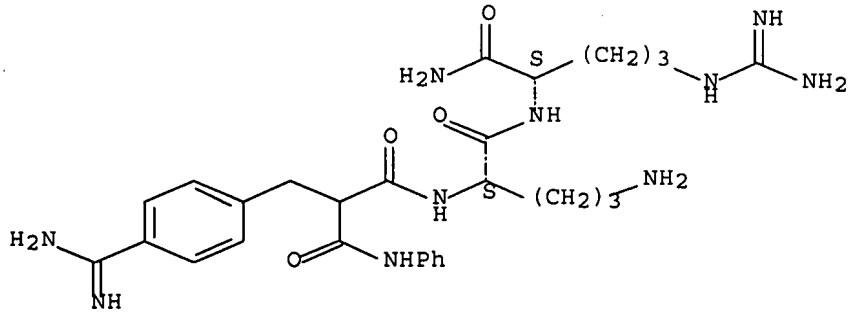


RN 356543-99-2 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-L-ornithyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

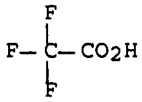
CRN 356543-98-1
CMF C28 H40 N10 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

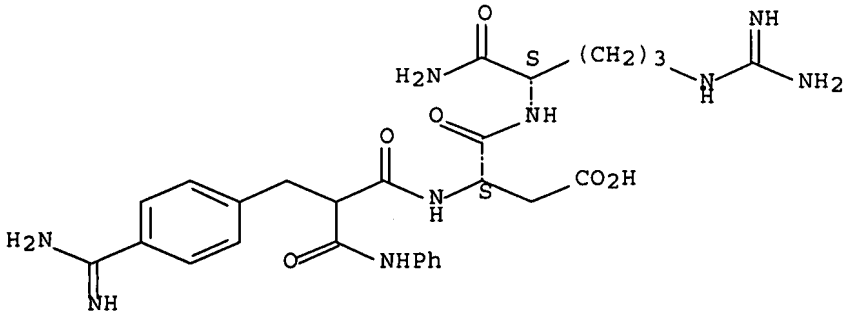


RN 356544-07-5 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-L-α-aspartyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

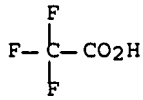
CRN 356544-06-4
CMF C27 H35 N9 O6

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

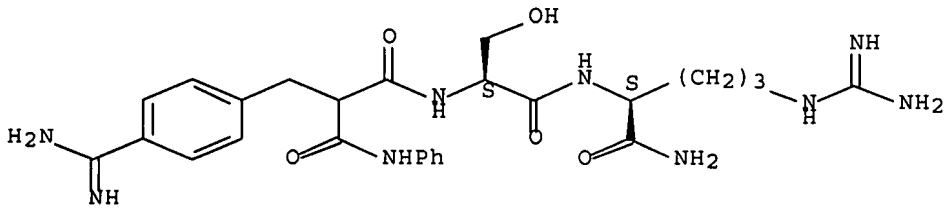


RN 356544-15-5 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-L-seryl-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

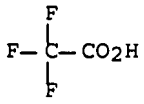
CRN 356544-14-4
CMF C26 H35 N9 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

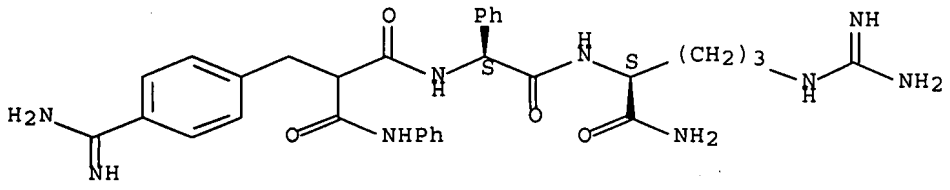


RN 356544-24-6 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-(2S)-2-phenylglycyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

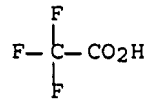
CRN 356544-23-5
CMF C31 H37 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

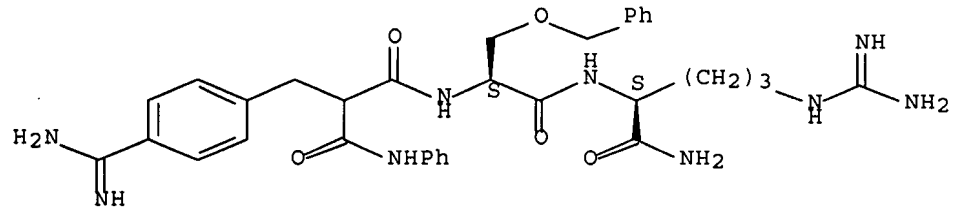


RN 356544-32-6 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-O-(phenylmethyl)-L-seryl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

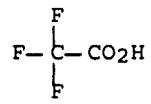
CRN 356544-31-5
CMF C33 H41 N9 O5

Absolute stereochemistry.



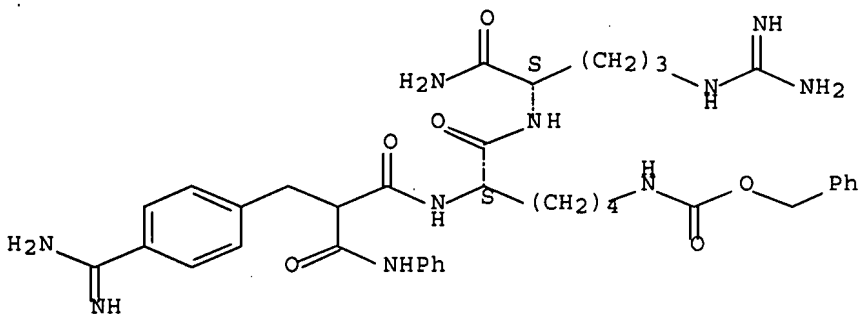
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 356544-36-0 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-N6-[(phenylmethoxy)carbonyl]-L-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

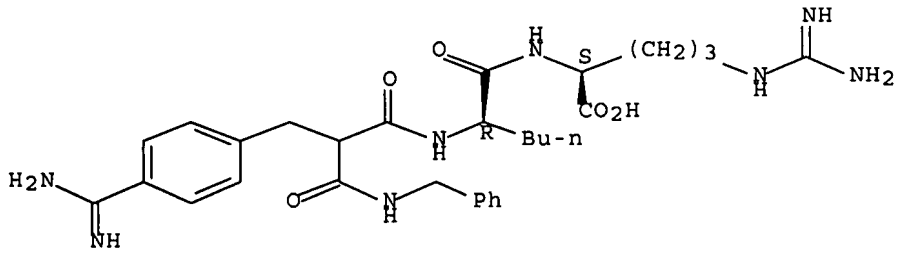


RN 356544-52-0 CAPLUS
CN L-Arginine, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-D-norleucyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

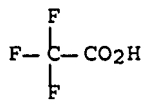
CRN 356544-51-9
CMF C30 H42 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

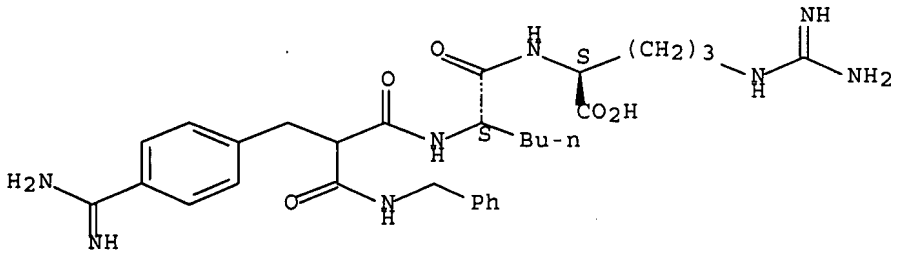


RN 356544-62-2 CAPLUS
CN L-Arginine, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-L-norleucyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

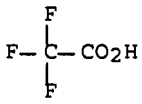
CRN 356544-61-1
CMF C30 H42 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

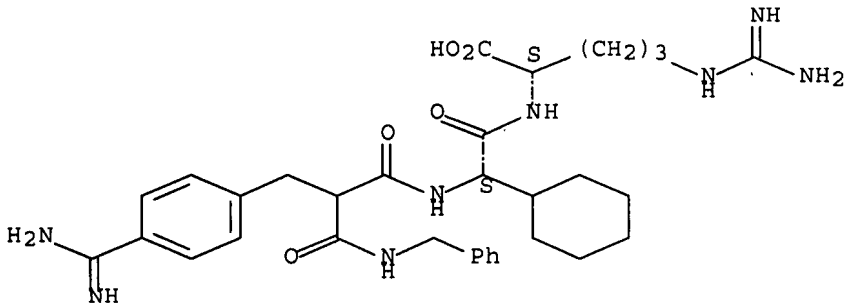


RN 356544-68-8 CAPLUS
CN L-Arginine, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

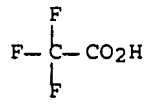
CRN 356544-67-7
CMF C32 H44 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

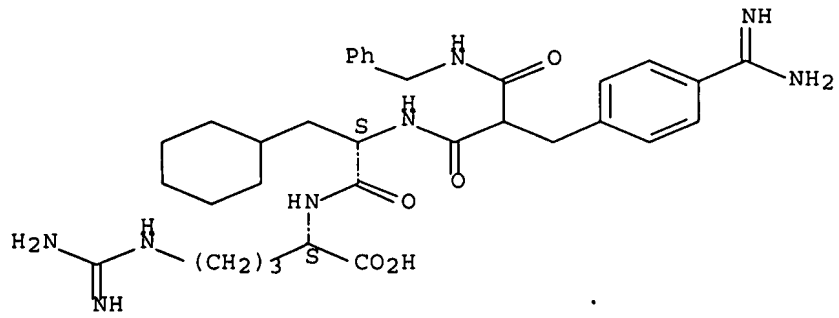


RN 356544-74-6 CAPLUS
CN L-Arginine, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-3-cyclohexyl-L-alanyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

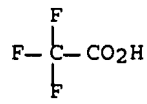
CRN 356544-73-5
CMF C33 H46 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



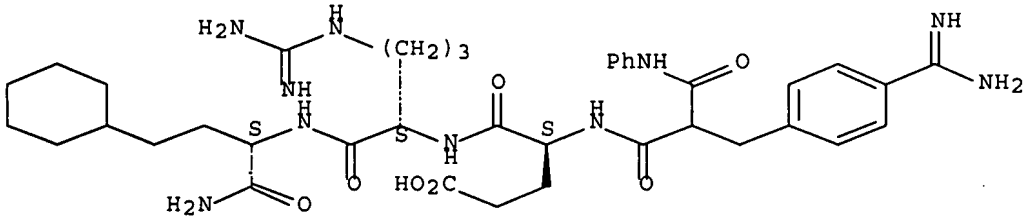
RN 356544-80-4 CAPLUS
CN Cyclohexanebutanamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-

phenyl-β-alanyl-L-α-glutamyl-L-arginyl-α-amino-,
(αS)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

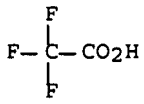
CRN 356544-79-1
CMF C38 H54 N10 O7

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

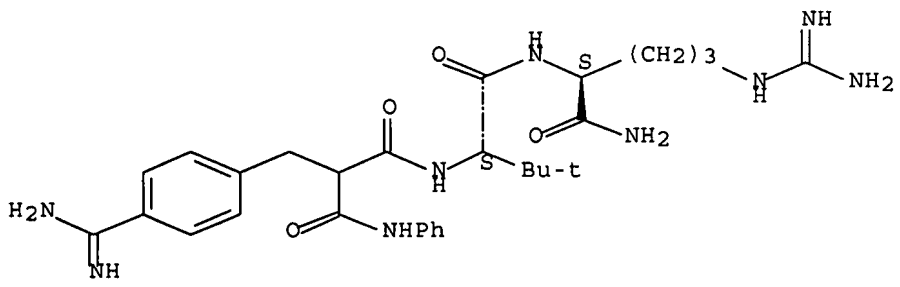


RN 356545-29-4 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-
β-alanyl-3-methyl-L-valyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

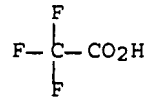
CRN 356545-28-3
CMF C29 H41 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

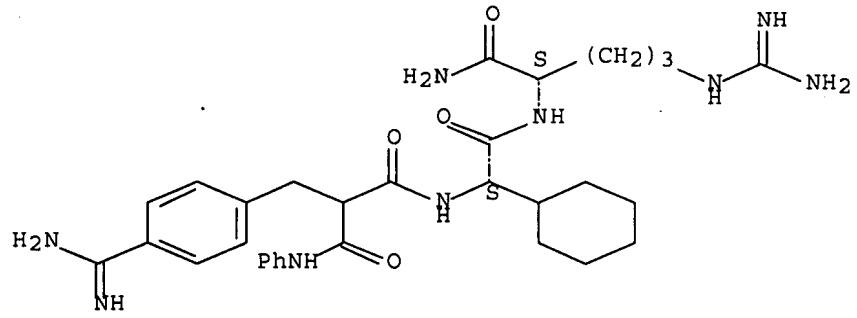


RN 356545-35-2 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

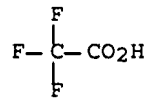
CRN 356545-34-1
CMF C31 H43 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

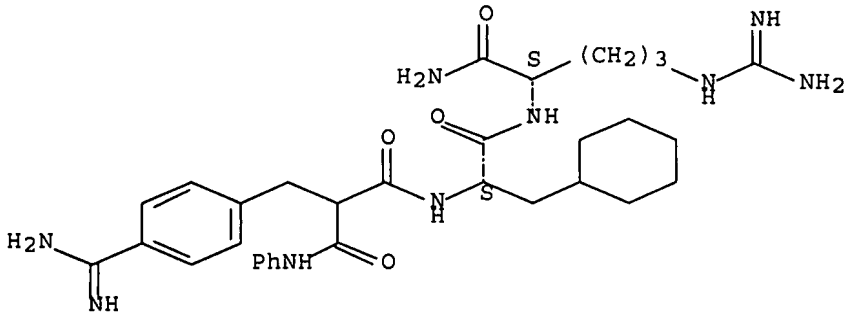


RN 356545-43-2 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-3-cyclohexyl-L-alanyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

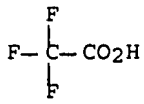
CRN 356545-42-1
CMF C32 H45 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

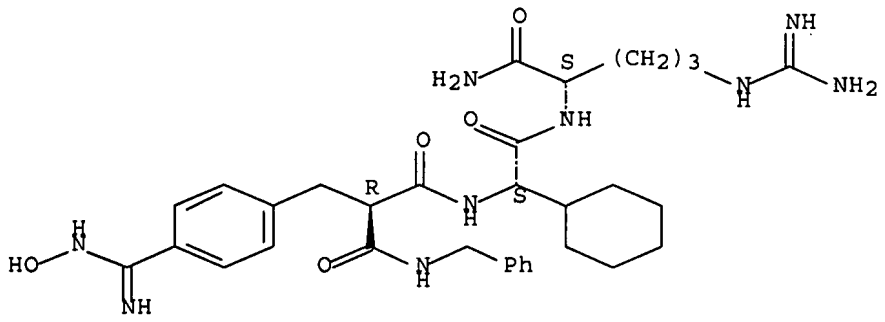


RN 356545-45-4 CAPLUS
CN L-Argininamide, (2R)-2-[[4-[(hydroxyamino)iminomethyl]phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

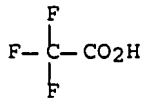
CRN 356545-44-3
CMF C32 H45 N9 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

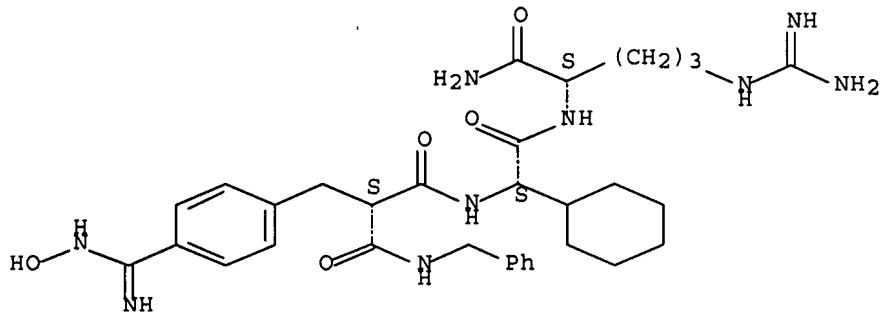


RN 356545-47-6 CAPLUS
CN L-Argininamide, (2S)-2-[[4-[(hydroxyamino)iminomethyl]phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

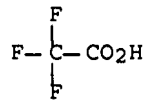
CRN 356545-46-5
CMF C32 H45 N9 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

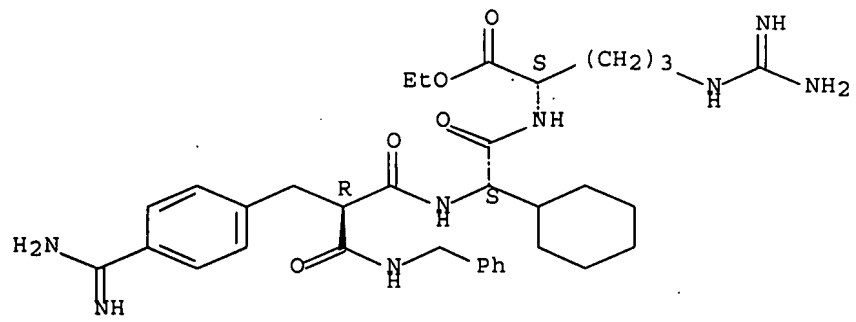


RN 356545-53-4 CAPLUS
CN L-Arginine, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, ethyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

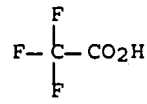
CRN 356545-52-3
CMF C34 H48 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

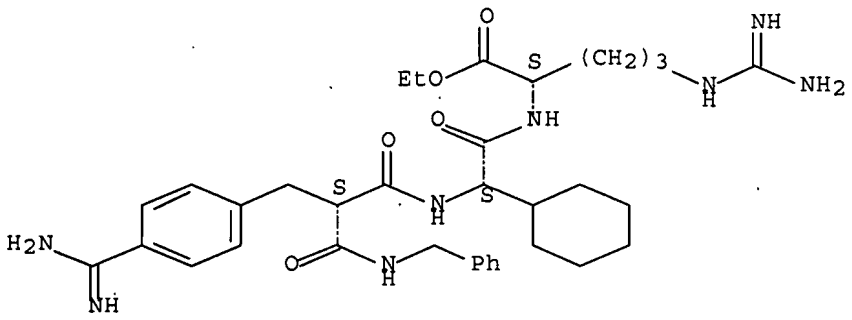


RN 356545-55-6 CAPLUS
CN L-Arginine, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, ethyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

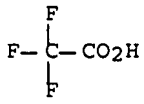
CRN 356545-54-5
CMF C34 H48 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

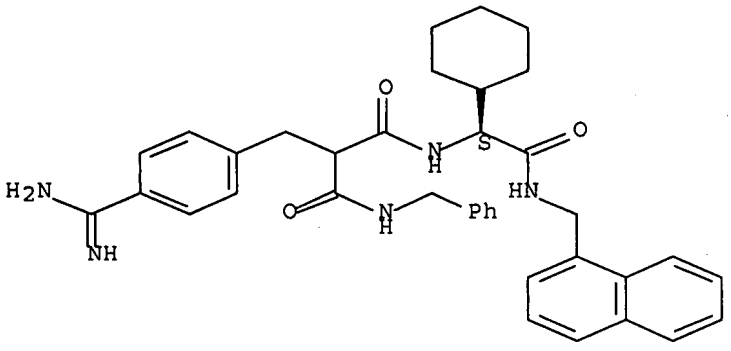


RN 356545-60-3 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-1-cyclohexyl-2-[(1-naphthalenylmethyl)amino]-2-oxoethyl]-N'-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

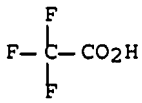
CRN 356545-59-0
CMF C37 H41 N5 O3

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

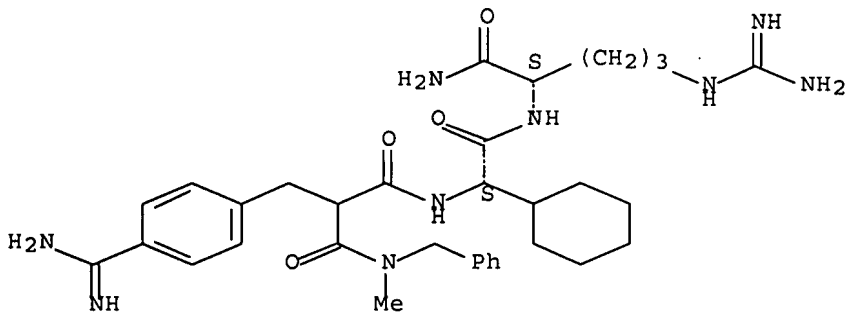


RN 356545-66-9 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

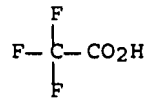
CRN 356545-65-8
CMF C33 H47 N9 O4

Absolute stereochemistry.



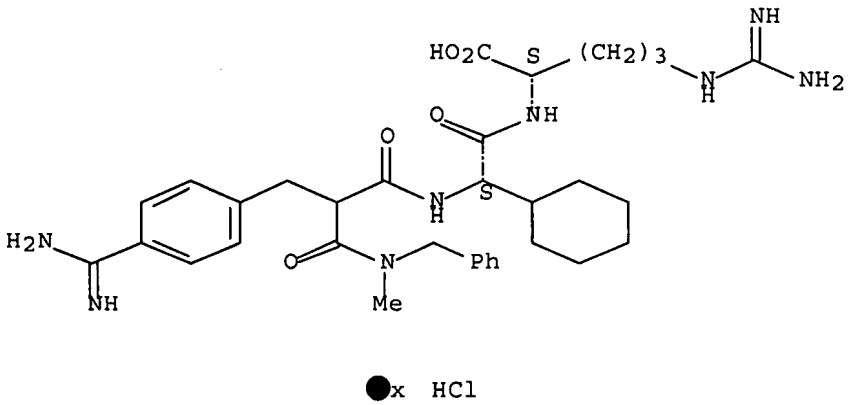
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 356545-67-0 CAPLUS
CN L-Arginine, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



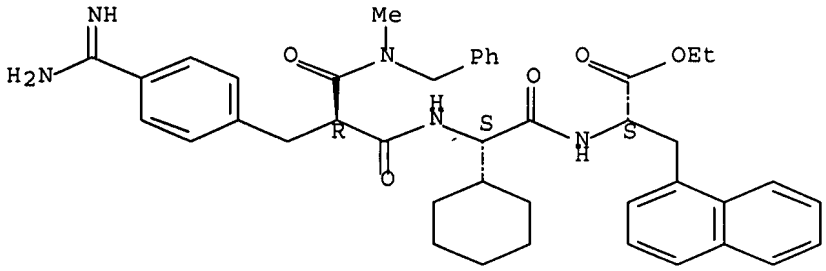
● x HCl

RN 356545-69-2 CAPLUS
CN L-Alanine, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-3-(1-naphthalenyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

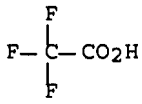
CRN 356545-68-1
CMF C42 H49 N5 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

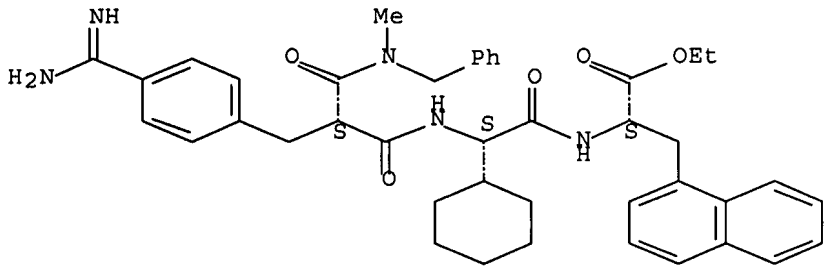


RN 356545-71-6 CAPLUS
CN L-Alanine, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-3-(1-naphthalenyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

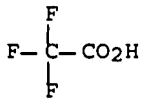
CRN 356545-70-5
CMF C42 H49 N5 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

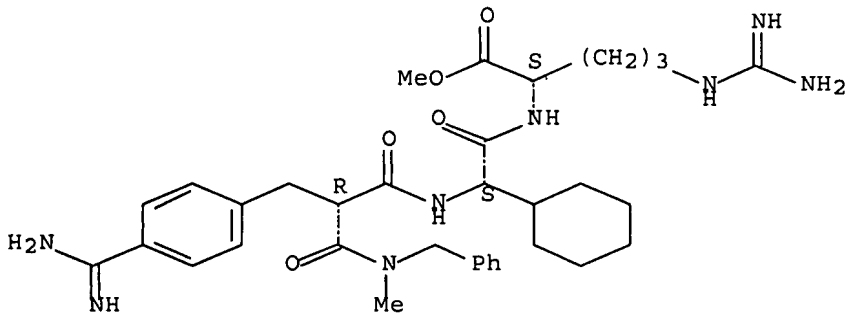


RN 356545-73-8 CAPLUS
CN L-Arginine, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, methyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

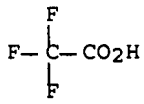
CRN 356545-72-7
CMF C34 H48 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

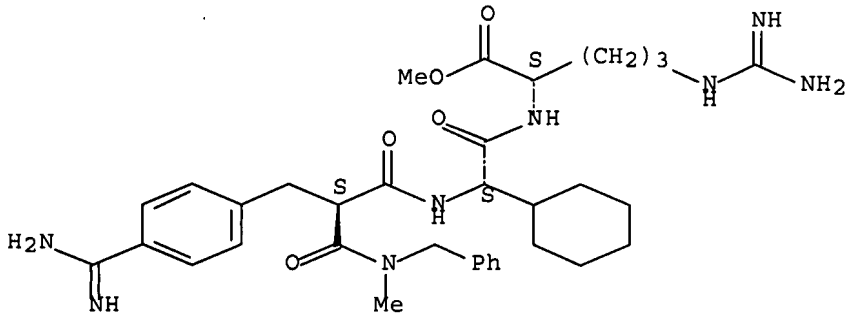


RN 356545-75-0 CAPLUS
CN L-Arginine, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, methyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

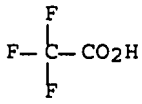
CRN 356545-74-9
CMF C34 H48 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

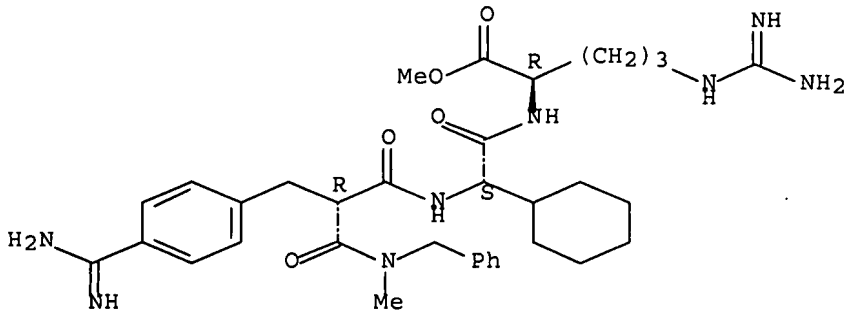


RN 356545-77-2 CAPLUS
CN D-Arginine, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, methyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

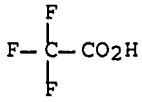
CRN 356545-76-1
CMF C34 H48 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

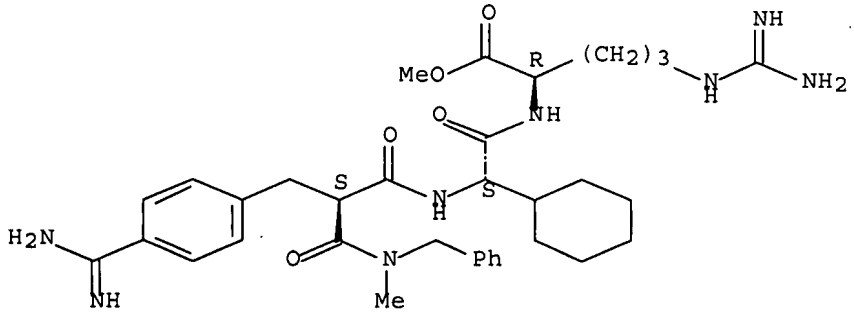


RN 356545-79-4 CAPLUS
CN D-Arginine, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, methyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

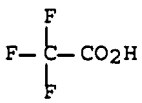
CRN 356545-78-3
CMF C34 H48 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

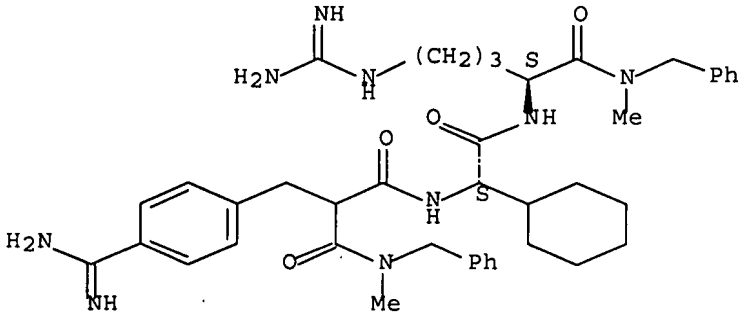


RN 356545-81-8 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-N-methyl-N-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

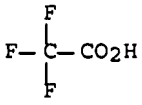
CRN 356545-80-7
CMF C41 H55 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

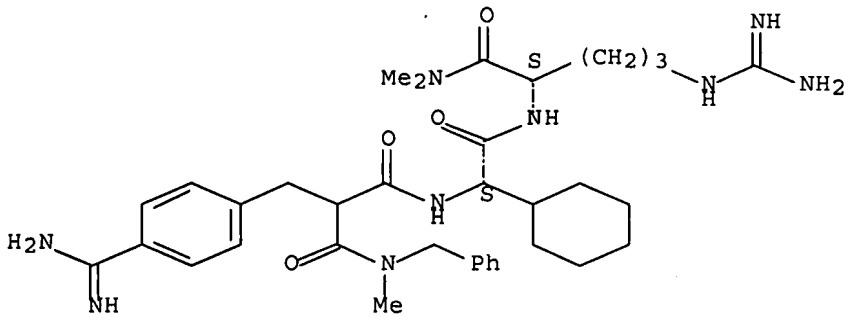


RN 356545-83-0 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-N,N-dimethyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

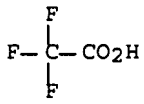
CRN 356545-82-9
CMF C35 H51 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

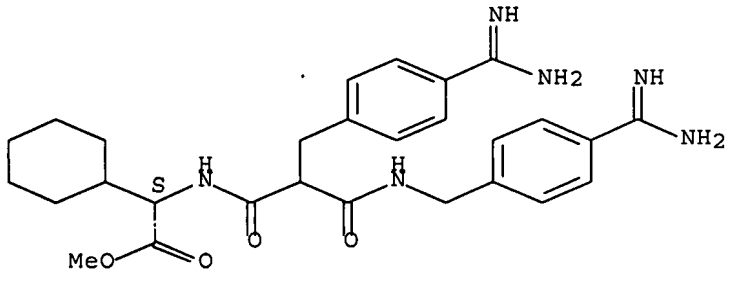


RN 356545-85-2 CAPLUS
CN Cyclohexaneacetic acid, α-[[2-[[4-(aminoiminomethyl)phenyl]methyl]-3-[[[4-(aminoiminomethyl)phenyl]methyl]amino]-1,3-dioxopropyl]amino]-, methyl ester, (αS)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356545-84-1
CMF C28 H36 N6 O4

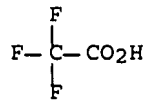
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2

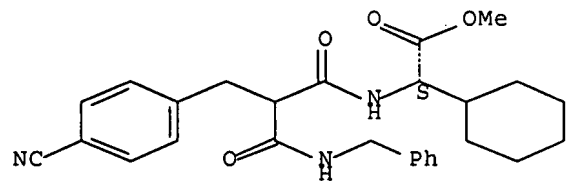


IT *280554-59-8P 280554-60-1P 280554-61-2P*
356545-90-9P 356545-91-0P 356545-92-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of malonic acid amide derivs. as inhibitors of blood clotting factor Xa)

RN 280554-59-8 CAPLUS

CN Cyclohexaneacetic acid, α-[[2-[(4-cyanophenyl)methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

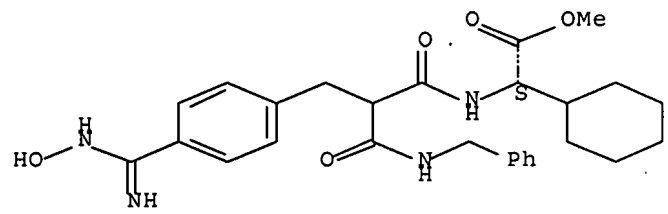
Absolute stereochemistry.



RN 280554-60-1 CAPLUS

CN Cyclohexaneacetic acid, α-[[2-[[4-[(hydroxyamino)iminomethyl]phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

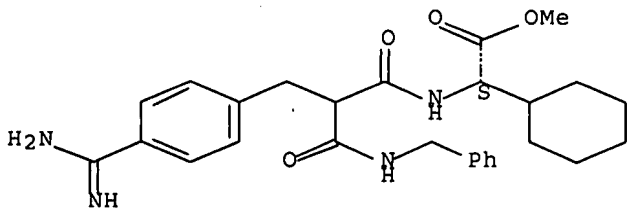
Absolute stereochemistry.



RN 280554-61-2 CAPLUS

CN Cyclohexaneacetic acid, α-[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

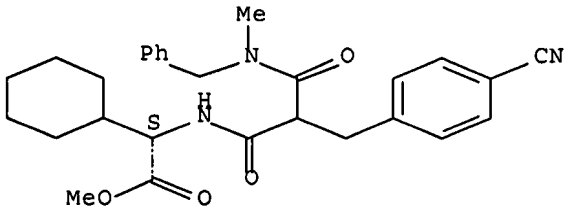
Absolute stereochemistry.



RN 356545-90-9 CAPLUS

CN Cyclohexaneacetic acid, α-[[2-[(4-cyanophenyl)methyl]-3-[methyl(phenylmethyl)amino]-1,3-dioxopropyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

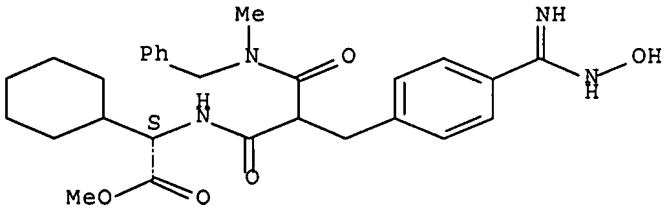
Absolute stereochemistry.



RN 356545-91-0 CAPLUS

CN Cyclohexaneacetic acid, α-[[2-[[4-[(hydroxyamino)iminomethyl]phenyl]methyl]-3-[methyl(phenylmethyl)amino]-1,3-dioxopropyl]amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

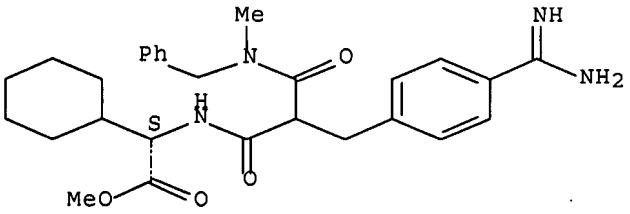
Absolute stereochemistry.



RN 356545-92-1 CAPLUS

CN Cyclohexaneacetic acid, α-[[2-[[4-(aminoiminomethyl)phenyl]methyl]-3-[methyl(phenylmethyl)amino]-1,3-dioxopropyl]amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

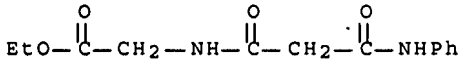


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 10 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:457054 CAPLUS Full-text
DOCUMENT NUMBER: 135:210602
TITLE: Versatile synthesis of malonamic acid derivatives from a β-ketothioester
AUTHOR(S): Lopez-Alvarado, P.; Avendano, C.; Carlos Menendez, J.
CORPORATE SOURCE: Facultad de Farmacia, Departamento de Quimica Organica y Farmaceutica, Universidad Complutense, Madrid, 28040, Spain
SOURCE: Tetrahedron Letters (2001), 42(27), 4479-4482
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:210602

AB An efficient synthetic route is described that allows the preparation under mild conditions of several types of malonamic acid derivs. The S-tert-Bu acetothioacetate monoanion reacted with aryl or alkyl isocyanates to give β-amidothioesters in one step and 73-87% yield, after spontaneous deacetylation of tricarbonyl intermediates. E.g., S-tert-Bu 3-oxothiobutanoate was reacted with cyclohexyl isocyanate to give S-tert-Bu cyclohexylcarbamoylthioacetate in 87% yield. Treatment of these thioesters with several aliphatic or aromatic alcs. and amines at room temperature in THF or DME and in the presence of silver trifluoroacetate provided, resp., the corresponding malonamic acid esters and malonamides in 80-100% yield.

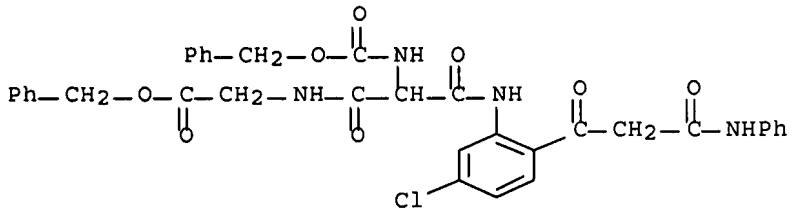
IT ***339274-38-3P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 339274-38-3 CAPLUS
CN Glycine, 3-oxo-N-phenyl-β-alanyl-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 11 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:278994 CAPLUS Full-text
DOCUMENT NUMBER: 135:107312
TITLE: Efficient synthesis of novel benzo-[e]-[1,4]-diazepine

derivatives
AUTHOR(S): Messeri, T.; Pentassuglia, G.; Di Fabio, R.
CORPORATE SOURCE: Medicines Research Center, GlaxoWellcome S.p.A., Verona, I-37135, Italy
SOURCE: Tetrahedron Letters (2001), 42(18), 3227-3230
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:107312
AB Following two efficient synthetic routes, a novel series of (2Z)-(8-chloro-1,2,3,4-tetrahydro-2-oxo-5H-1,4-benzodiazepin-5-ylidene)-N- phenylacetamide derivs. (bearing an unusual Z exo-methylencarbamoyl side chain at the C-5 position) were prepared to identify new antagonists of the glycine binding site associated with NMDA receptor. Pharmacol. test data were not reported.
IT ***350238-05-0P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (2Z)-(8-chloro-1,2,3,4-tetrahydro-2-oxo-5H-1,4-benzodiazepin-
5-ylidene)-N-phenylacetamide derivs.)
RN 350238-05-0 CAPLUS
CN Glycine, 3-[[5-chloro-2-[1,3-dioxo-3-(phenylamino)propyl]phenyl]amino]-3-oxo-N-[(phenylmethoxy)carbonyl]alanyl-, phenylmethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 12 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:133356 CAPLUS Full-text
DOCUMENT NUMBER: 134:352962
TITLE: A general, high-yielding synthesis of β-diamides and β-amido esters
AUTHOR(S): Lopez-Alvarado, Pilar; Avendano, Carmen; Menendez, J. Carlos
CORPORATE SOURCE: Departamento de Quimica Organica y Farmaceutica, Facultad de Farmacia, Universidad Complutense, Madrid, 28040, Spain
SOURCE: Proceedings of ECSOC-3, [and] Proceedings of ECSOC-4, Sept. 1-30, 1999 and 2000 (2000), Meeting Date 1999-2000, 751-754. Editor(s): Pombo-Villar, Esteban. Molecular Diversity Preservation International: Basel, Switz.
CODEN: 69AXZT
DOCUMENT TYPE: Conference; (computer optical disk)
LANGUAGE: English

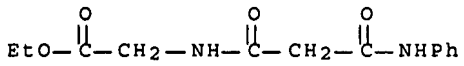
OTHER SOURCE(S): CASREACT 134:352962

AB An electronic conference report on a new and efficient synthetic route to malonamides and malonamic acid esters. S-tert-Bu acetothioacetate monoanion reacted with aryl or alkyl isocyanates to give tricarbonyl compds., which spontaneously deacetylated to the corresponding β-amido thioesters. Treatment of the latter with aliphatic or aromatic amines or alcs. at room temperature in the presence of silver trifluoroacetate provided malonamides or malonamic acid esters, resp., in excellent overall yields.

IT ***339274-38-3P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of β-diamides and β-amido esters)

RN 339274-38-3 CAPLUS

CN Glycine, 3-oxo-N-phenyl-β-alanyl-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 13 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:653161 CAPLUS Full-text

DOCUMENT NUMBER: 134:5141

TITLE: Replacement of glycine with dicarbonyl and related moieties in analogs of the C-terminal pentapeptide of cholecystokinin: CCK2 agonists displaying a novel binding mode

AUTHOR(S): Bellier, Bruno; Million, Marie-Emmanuelle; DaNascimento, Sophie; Meudal, Herve; Kellou, Safia; Maigret, Bernard; Garbay, Christiane

CORPORATE SOURCE: Departement de Pharmacochimie Moleculaire et Structurale, U266 INSERM UMR 8600 CNRS, UFR des Sciences Pharmaceutiques et Biologiques, Paris, 75270, Fr.

SOURCE: Journal of Medicinal Chemistry (2000), 43(20), 3614-3623
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:5141

AB Recent advances in the field of cholecystokinin have indicated the possible occurrence of multiple affinity states of the CCK2 receptor. Besides, numerous pharmacol. expts. performed "in vitro" and "in vivo" support the eventuality of different pharmacol. profiles associated to CCK2 ligands. Indeed, some agonists are essentially anxiogenic and ineffective in memory tests, whereas others are not anxiogenic and appear as able to reinforce memory. The reference compound for the latter profile is the CCK-8 analog BC 264 (Boc-Tyr(SO3H)-gNle-mGly-Trp-(NMe)Nle-Asp-Phe-NH2). However, although tetrapeptide ligands based on CCK-4 (Trp-Met-Asp-Phe-NH2) are known to possess sufficient structural features for CCK2 recognition, none shares the properties of BC 264. Hence we have developed new short peptidic or pseudo-peptidic derivs. containing the C-terminal tetrapeptide of BC 264. Our results indicate that some compds. characterized by the presence of two carbonyl groups at the N-terminus, as in (HO2C-CH2-CONH-Trp-(NMe)Nle-Asp-Phe-NH2), are likely to show a

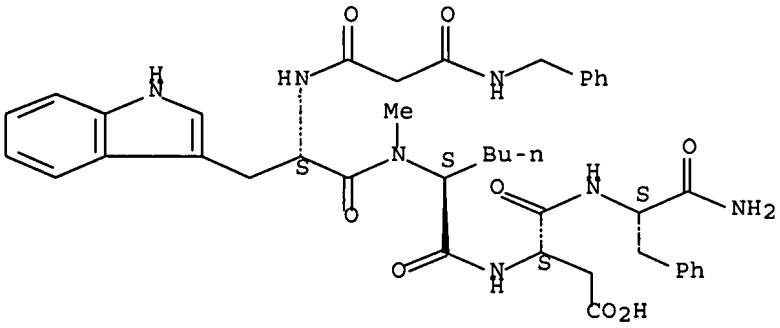
BC 264-like profile, bind to the CCK2 receptor in a specific way, and display remarkable affinities (0.28 nM on guinea-pig cortex membrane prepns.). This original binding mode is discussed and further enlightened by NMR and mol. modeling studies.

IT *203563-93-3P*
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of pseudopeptides as CCK2 agonists by replacement of glycine with dicarbonyl in C-terminal pentapeptides)

RN 203563-93-3 CAPLUS

CN L-Phenylalaninamide, 3-oxo-N-(phenylmethyl)-β-alanyl-L-tryptophyl-N-methyl-L-norleucyl-L-α-aspartyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

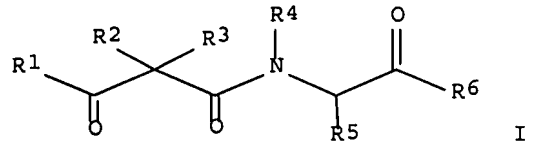
L53 ANSWER 14 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:456736 CAPLUS Full-text
DOCUMENT NUMBER: 133:89228
TITLE: Novel malonic acid derivatives, processes for their preparation, their use and pharmaceutical compositions containing them (inhibition of factor Xa activity)
INVENTOR(S): Defossa, Elisabeth; Heinelt, Uwe; Klingler, Otmar; Zoller, Gerhard; Matter, Hans; Al-Obeidi, Fahad A.; Walser, Armin; Wildgoose, Peter
PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany
SOURCE: Eur. Pat. Appl., 76 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1016663	A1	20000705	EP 1999-100002	19990102
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CA 2358578	A1	20000713	CA 1999-2358578	19991223
WO 2000040571	A1	20000713	WO 1999-EP10340	19991223
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,				

CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

BR 9916732	A	20010925	BR 1999-16732		19991223
EP 1140878	A1	20011010	EP 1999-964667		19991223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
TR 200101903	T2	20011121	TR 2001-200101903		19991223
HU 200105437	A2	20020529	HU 2001-5437		19991223
JP 2002534420	T	20021015	JP 2000-592279		19991223
US 6395737	B1	20020528	US 1999-473053		19991228
ZA 2001004770	A	20020612	ZA 2001-4770		20010612
NO 2001002983	A	20010615	NO 2001-2983		20010615
IN 2001CN00908	A	20050304	IN 2001-CN908		20010628
PRIORITY APPLN. INFO.:			EP 1999-100002	A	19990102
			EP 1999-119537	A	19991001
			WO 1999-EP10340	W	19991223

OTHER SOURCE(S): MARPAT 133:89228
GI



I

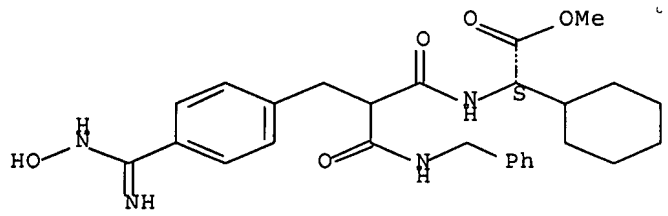
AB The present invention relates to the preparation of new compds. for the inhibition of blood clotting proteins, and more particularly, to malonic acid derivs., I (R1 = organoamino, organoalkoxy, etc.; R2 = H, C1-4 alkyl; R3 = (un)substituted C6-10-aryl-C1-4-alkyl; R4 = H, C1-4-alkyl, C3-7-cycloalkyl, C3-7-cycloalkyl-C1-4-alkyl, C6-10-aryl-C1-4-alkyl; R5 = H, C1-10-alkyl, C3-7-cycloalkyl, C3-7-cycloalkyl-C1-4-alkyl, C6-10-aryl, C6-10-aryl-C1-4-alkyl, etc.; R4R5 = cyclic hydrocarbyl; R6 = organoalkoxy, organoamino, etc.). Thus, 2-(R,S)-(4-carbamimidoylbenzyl)-N-[(S)- cyclohexyl(piperidin-4-ylcarbamoyl)methyl]-N',N'-dimethylmalonamide acetic acid salt was prepared in several steps starting from 2,2- dimethyl[1,3]dioxane-4,6-dione and 4-formylbenzonitrile. I are inhibitors (activity given) of the blood clotting enzyme factor Xa. The invention also relates to processes for the preparation of I, to methods of inhibiting factor Xa activity and of inhibiting blood clotting, to the use of I in the treatment and prophylaxis of diseases, which can be treated or prevented by the inhibition of factor Xa activity such as thromboembolic diseases, and to the use of the compds. I in the preparation of medicaments to be applied in such diseases. The invention further relates to compns. containing I in admixt. or otherwise in association with an inert carrier, in particular pharmaceutical compns. containing a compound of formula I together with pharmaceutically acceptable carrier substances and auxiliary substances.

IT *280554-60-1P*
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and catalytic hydrogenation of)

RN 280554-60-1 CAPLUS

CN Cyclohexaneacetic acid, α-[[2-[[4-[(hydroxyamino)iminomethyl]phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



IT *280553-84-6P*

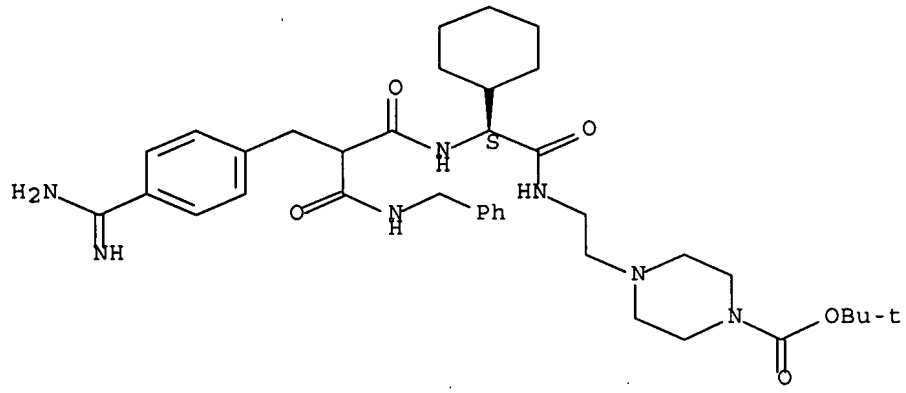
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with benzylcarbamoyl carbamimidoylphenylpropionyla mino cyclohexylacetic acid salt)

RN 280553-84-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[2-[[(2S)-[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]cyclohexylacetyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT *280554-61-2P*

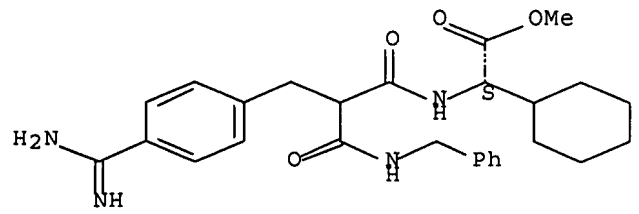
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with hydrochloric acid)

RN 280554-61-2 CAPLUS

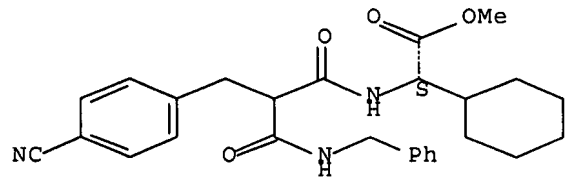
CN Cyclohexaneacetic acid, α-[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



IT *280554-59-8P*
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with hydroxylamine)
RN 280554-59-8 CAPLUS
CN Cyclohexaneacetic acid, α-[[2-[(4-cyanophenyl)methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

Absolute stereochemistry.

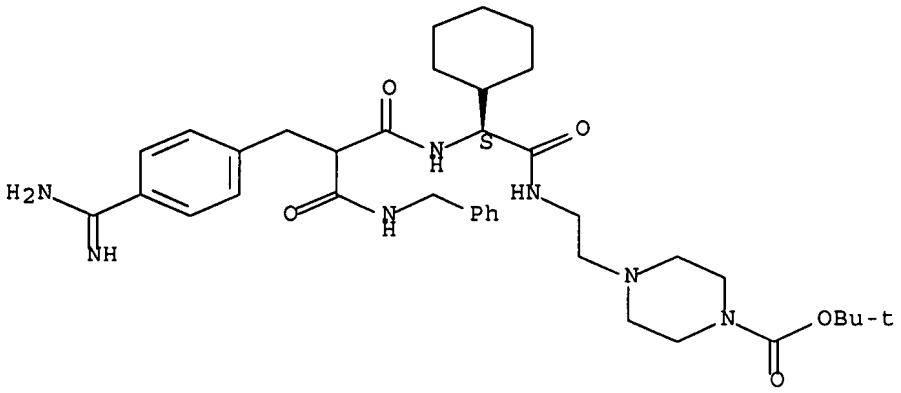


IT *280553-85-7P*
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of novel malonic acid derivs. as factor Xa inhibitors)
RN 280553-85-7 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[2-[[(2S)-[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]cyclohexylacetyl]amino]ethyl]-, 1,1-dimethylethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

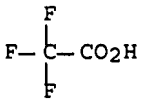
CRN 280553-84-6
CMF C37 H53 N7 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

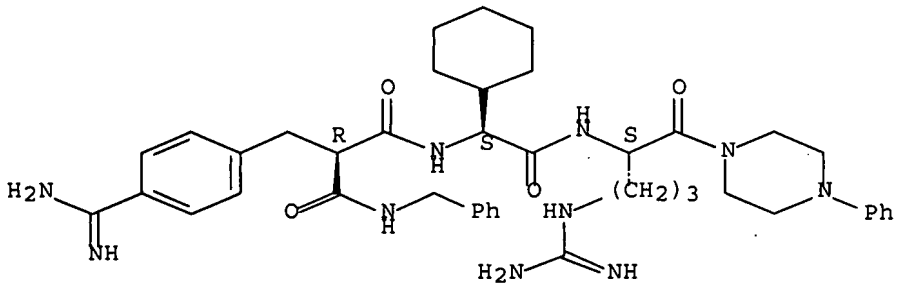


IT *280553-80-2P 280553-83-5P 280553-87-9P*
280553-91-5P 280553-96-0P 280554-05-4P
280554-06-5P 280554-33-8P 280554-35-0P
280554-37-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel malonic acid derivs. as factor Xa inhibitors)
RN 280553-80-2 CAPLUS
CN Glycinamide, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(4-phenyl-1-piperazinyl)carbonyl]butyl]-2-cyclohexyl-, (2S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

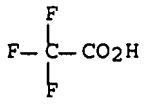
CRN 280553-79-9
CMF C42 H56 N10 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

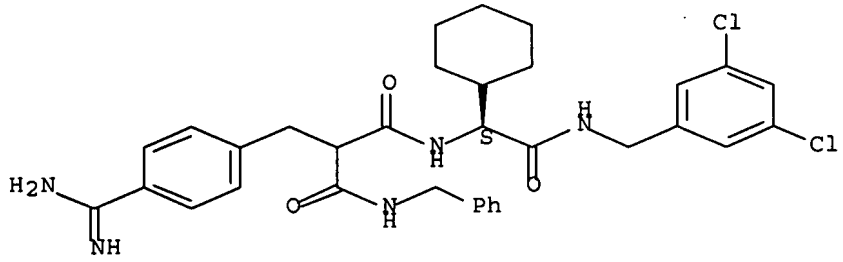


RN 280553-83-5 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-1-cyclohexyl-2-[[(3,5-dichlorophenyl)methyl]amino]-2-oxoethyl]-N'-(phenylmethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 280553-82-4
CMF C33 H37 Cl2 N5 O3

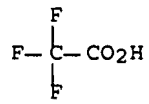
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2

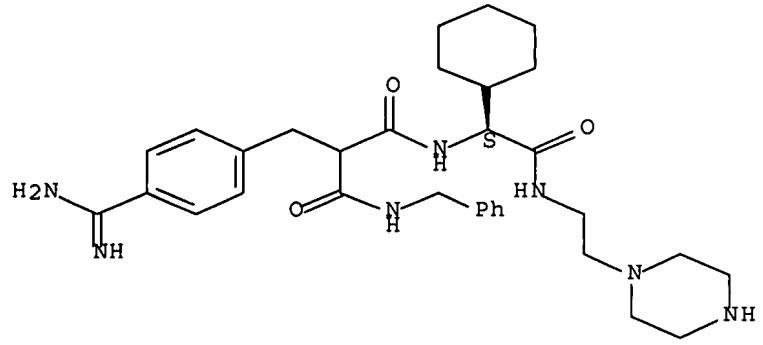


RN 280553-87-9 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-1-cyclohexyl-2-oxo-2-[[2-(1-piperazinyl)ethyl]amino]ethyl]-N'-(phenylmethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

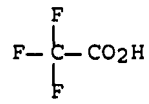
CRN 280553-86-8
CMF C32 H45 N7 O3

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

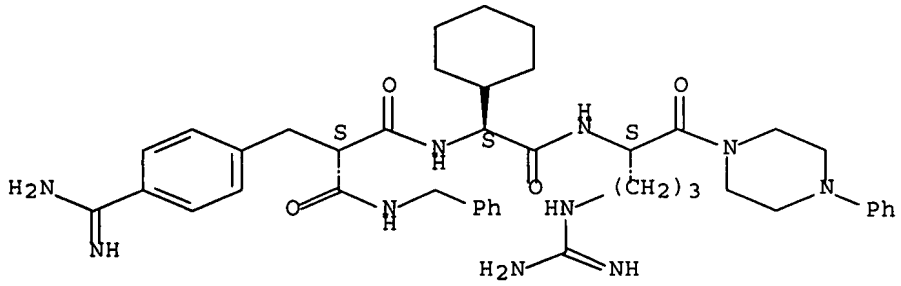


RN 280553-91-5 CAPLUS
CN Glycinamide, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(4-phenyl-1-piperazinyl)carbonyl]butyl]-2-cyclohexyl-, (2S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

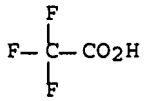
CRN 280553-90-4
CMF C42 H56 N10 O4

Absolute stereochemistry.



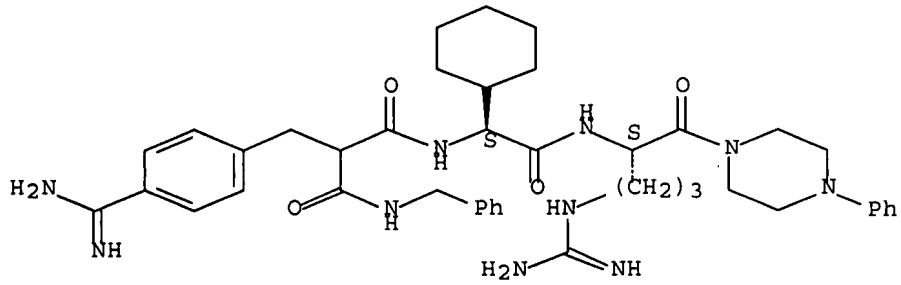
CM 2

CRN 76-05-1
CMF C2 H F3 O2



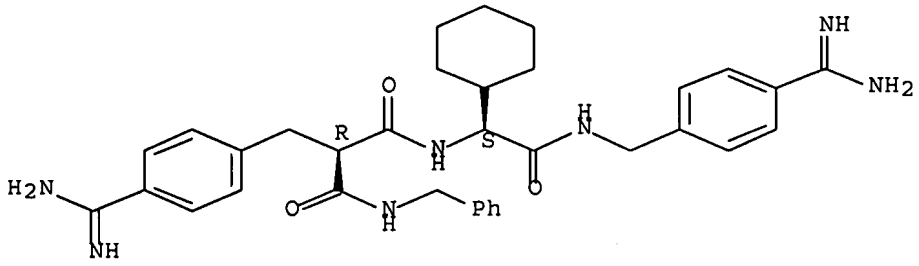
RN 280553-96-0 CAPLUS
CN Glycinamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(4-phenyl-1-piperazinyl)carbonyl]butyl]-2-cyclohexyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



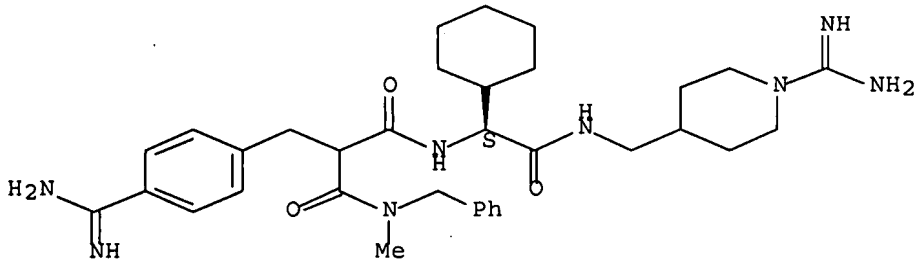
RN 280554-05-4 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-2-[[[4-(aminoiminomethyl)phenyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N'-(phenylmethyl)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 280554-06-5 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N'-[(1S)-2-[[[1-(aminoiminomethyl)-4-piperidinyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

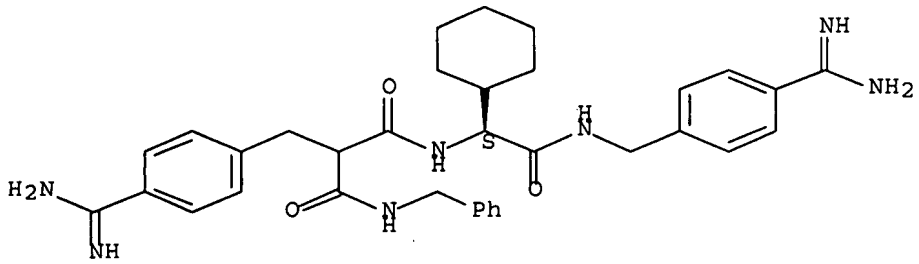


RN 280554-33-8 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-2-[[[4-(aminoiminomethyl)phenyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N'-(phenylmethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

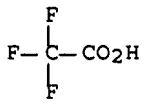
CRN 280554-32-7
CMF C34 H41 N7 O3

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

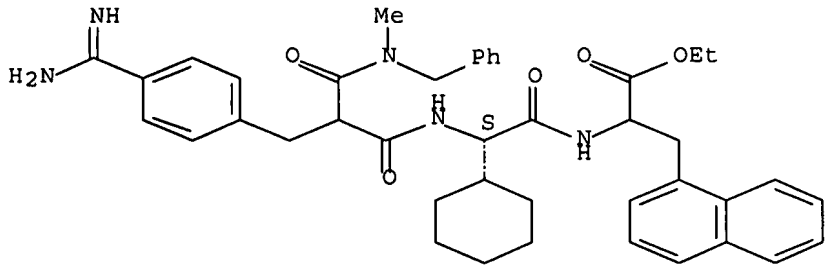


RN 280554-35-0 CAPLUS
CN Alanine, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-3-(1-naphthalenyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

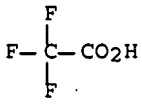
CRN 280554-34-9
CMF C42 H49 N5 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

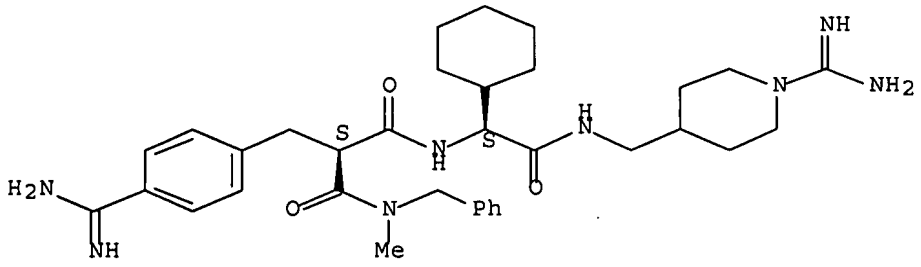


RN 280554-37-2 CAPLUS
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N'-[(1S)-2-[[[1-(aminoiminomethyl)-4-piperidinyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N-methyl-N-(phenylmethyl)-, (2S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

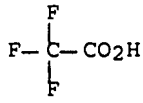
CRN 280554-36-1
CMF C34 H48 N8 O3

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 15 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:421088 CAPLUS Full-text
DOCUMENT NUMBER: 133:58615
TITLE: Substituted aryl and heteroaryl derivatives of benzamidine and their use as antithrombics

INVENTOR(S): Priepke, Henning; Kauffmann, Iris; Hauel, Norbert; Ries, Uwe; Nar, Herbert; Stassen, Jean Marie; Wienen, Wolfgang

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma Kg, Germany

SOURCE: PCT Int. Appl., 178 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2000035859	A1	20000622	WO 1999-EP9921		19991213
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
DE 19858029	A1	20000621	DE 1998-19858029		19981216
DE 19948101	A1	20010412	DE 1999-19948101		19991007
CA 2353151	A1	20000622	CA 1999-2353151		19991213
EP 1140802	A1	20011010	EP 1999-965464		19991213
EP 1140802	B1	20040317			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
JP 2002532460	T	20021002	JP 2000-588121		19991213
JP 3827530	B2	20060927			
AT 261934	T	20040415	AT 1999-965464		19991213
US 6479524	B1	20021112	US 2001-868428		20011018
PRIORITY APPLN. INFO.:			DE 1998-19858029	A	19981216
			DE 1999-19948101	A	19991007
			WO 1999-EP9921	W	19991213

OTHER SOURCE(S): MARPAT 133:58615

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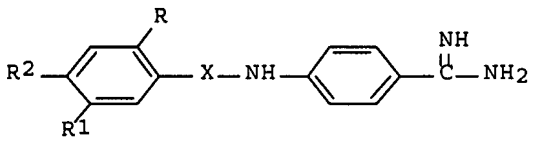


I

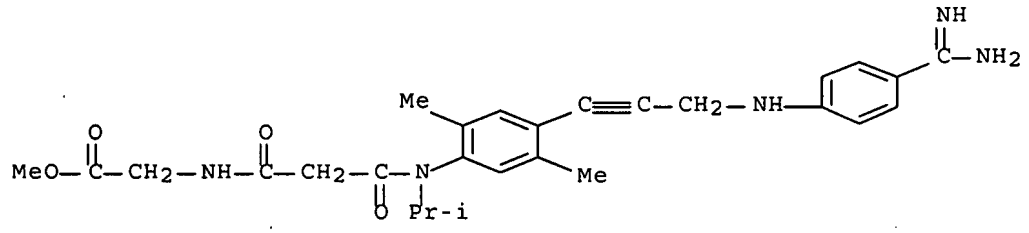
AB Aryl and heteroaryl derivs. of benzamidine Ar-A-HCR1-X-Y, such as I [R = Me, H; R1 = CH2CO2Me, Me; R2 = 2-methylpyrrolidinocarbonyl, COCHMe2, N-methyl-N-2-pyridylcarbonyl, pyrrolidinocarbonyl, N(CO2Et)CH2CH2CO2Me, N(CHMe2)NHCH2CO2H, N(CHMe2)COCH2CO2H; X = CH2C.tplbond.C, (CH2)3] were prepared for use as antithrombics. Thus, I [R = Me, R1 = CH2CO2Me, R2 = 2-methylpyrrolidinocarbonyl, X = CH2C.tplbond.C, II] was prepared from the

propargylbenzamidine and pyrrolidinocarbonylphenyl bromide fragments. II had an ED200 in the a-PTT time of 0.23 μM.

IT *276678-81-0P*
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted aryl and heteroaryl derivs. of benzamidine and their use as antithrombics)

RN 276678-81-0 CAPLUS

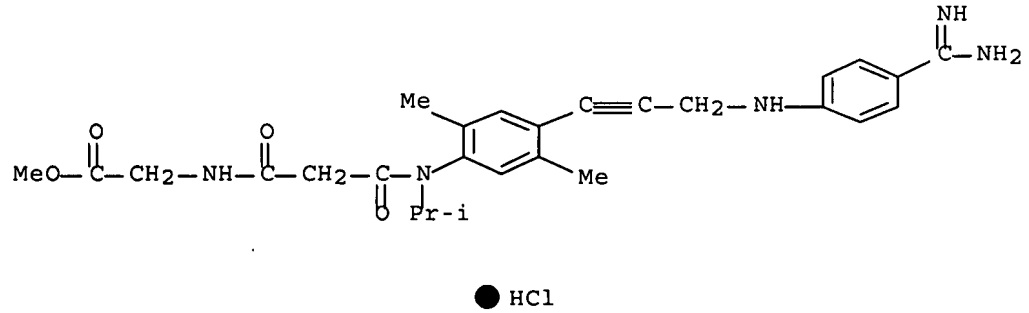
CN Glycine, N-[4-[3-[[4-(aminoiminomethyl)phenyl]amino]-1-propynyl]-2,5-dimethylphenyl]-N-(1-methylethyl)-3-oxo-β-alanyl-, methyl ester (9CI) (CA INDEX NAME)



IT *276676-53-0P*
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted aryl and heteroaryl derivs. of benzamidine and their use as antithrombics)

RN 276676-53-0 CAPLUS

CN Glycine, N-[4-[3-[[4-(aminoiminomethyl)phenyl]amino]-1-propynyl]-2,5-dimethylphenyl]-N-(1-methylethyl)-3-oxo-β-alanyl-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 16 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:53681 CAPLUS Full-text
DOCUMENT NUMBER: 132:108302
TITLE: Preparation of CS-1 peptidomimetics and their compositions
INVENTOR(S): Arrhenius, Thomas S.; Elices, Mariano J.; Gaeta,

Federico C. A.; He, Ya-Bo; Huyghe, Bernard G.; Chen, Paul G.
PATENT ASSIGNEE(S): Cytel Corporation, USA
SOURCE: PCT Int. Appl., 266 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000002903	A1	20000120	WO 1998-US26605	19981215
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9919153	A	20000201	AU 1999-19153	19981215
PRIORITY APPLN. INFO.:			US 1998-113689 A	19980710
			WO 1998-US26605 W	19981215

OTHER SOURCE(S): MARPAT 132:108302

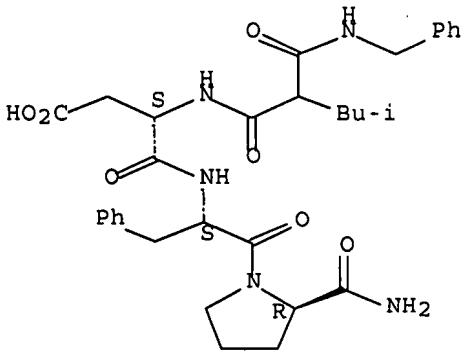
AB Peptidomimetics R1CONR2CHR3CONR4CH(CONR5R6)CH2CO2H [R1 = alkyl, aminoalkyl, or a ring structure which may form at R1, between R1 and R2 or between R1 and R4; R2 = H, alkyl, phenylalkyl or R2 and R1 form the R1 ring structure group; R3 = alkyl, alkyl alc., thioalkyl, dialkyl thioether, or a ring structure; R4 = H or R4 and R1 form the R1 ring structure; R5 = H or R5 and R6 form a ring structure; R6 = benzyl, an optionally substituted 5-, 6-, or 7-membered heterocyclic ring containing 1 or 2 nitrogen atoms, a pyridobenzazepine moiety, or a group CHR7CO-AR8R9 (A = N and R7, R8, R9 = alkyl, a ring structure, etc. or A = O and R7 = alkyl, a ring structure, etc., R8 = alkyl, and R9 is absent)] were prepared as inhibitors of the binding between the VLA-4 receptor and the fibronectin CS-1 domain. Thus, N-phenylacetyl-L-Leu-Asp-Phe-D-Pro-NH2 was prepared and assayed for binding inhibition potency (313 relative to a standard compound).

IT ***209601-97-8P 209602-44-8P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of CS-1 peptidomimetics and their compns.)

RN 209601-97-8 CAPLUS

CN D-Prolinamide, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)-β-alanyl-L-α-aspartyl-L-phenylalanyl- (9CI) (CA INDEX NAME)

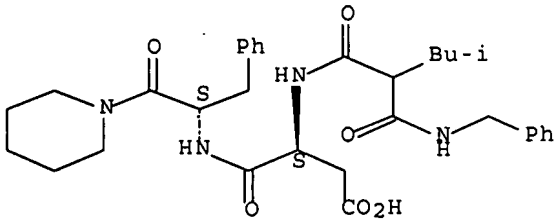
Absolute stereochemistry.



RN 209602-44-8 CAPLUS

CN L-α-Asparagine, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-2-oxo-1-(phenylmethyl)-2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 17 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:505686 CAPLUS Full-text

DOCUMENT NUMBER: 131:139496

TITLE: Fibronectin CS-1 peptidomimetics for inhibiting binding of CS-1 to VLA-4 and for treating immunoinflammatory conditions

INVENTOR(S): Arrhenius, Thomas S.; Elices, Mariano J.; Gaeta, Federico C. A.

PATENT ASSIGNEE(S): Cytel Corporation, USA

SOURCE: U.S., 81 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5936065	A	19990810	US 1995-462424	19950605
CA 2177840	A1	19950615	CA 1994-2177840	19941205
CN 1142832	A	19970212	CN 1994-194969	19941205
US 5688913	A	19971118	US 1995-435286	19950505
US 6117840	A	20000912	US 1997-837154	19970414

US 6103870 A 20000815 US 1997-923026 19970903
PRIORITY APPLN. INFO.: US 1993-164101 B2 19931206
US 1994-349024 B2 19941202
US 1995-435286 A1 19950505

OTHER SOURCE(S): MARPAT 131:139496

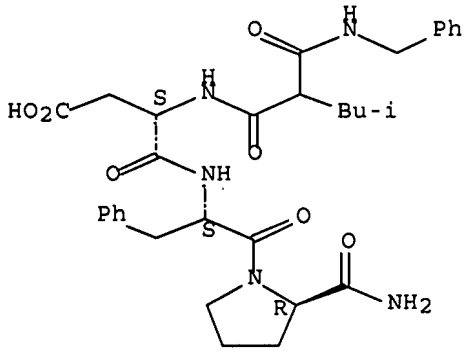
AB Peptidomimetic compds. are disclosed that inhibit the binding between the VLA-4 and the fibronectin CS-1 compound Pharmaceutical compns. containing a contemplated compound and methods for treating immunoinflammatory conditions using the compound are also disclosed.

IT *209601-97-8 209602-44-8*
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fibronectin CS-1 peptidomimetics for inhibiting binding of CS-1 to VLA-4 and for treating immunoinflammatory conditions)

RN 209601-97-8 CAPLUS

CN D-Prolinamide, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)-β-alanyl-L-α-aspartyl-L-phenylalanyl- (9CI) (CA INDEX NAME)

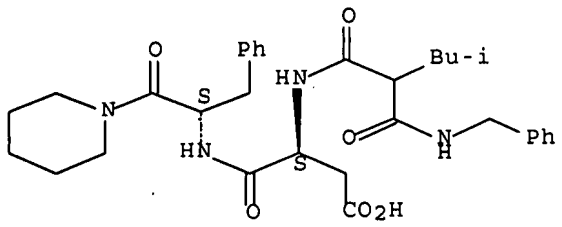
Absolute stereochemistry.



RN 209602-44-8 CAPLUS

CN L-α-Asparagine, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-2-oxo-1-(phenylmethyl)-2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



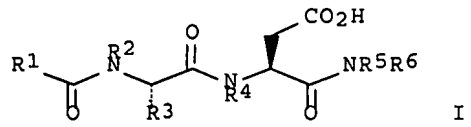
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 18 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:668012 CAPLUS Full-text
DOCUMENT NUMBER: 129:290438
TITLE: Preparation of CS-1 peptidomimetics and their compositions
INVENTOR(S): Arrhenius, Thomas S.; Elices, Mariano J.; Gaeta, Federico C. A.
PATENT ASSIGNEE(S): Cytel Corp., USA
SOURCE: U.S., 81 pp., Cont.-in-part of U.S. Ser. No. 349,024.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5821231	A	19981013	US 1995-461056	19950605
CA 2177840	A1	19950615	CA 1994-2177840	19941205
CN 1142832	A	19970212	CN 1994-194969	19941205
US 5688913	A	19971118	US 1995-435286	19950505
US 6117840	A	20000912	US 1997-837154	19970414
US 6103870	A	20000815	US 1997-923026	19970903
PRIORITY APPLN. INFO.:			US 1993-164101	B2 19931206
			US 1994-349024	A2 19941202
			US 1995-435286	A1 19950505

OTHER SOURCE(S): MARPAT 129:290438
GI



I

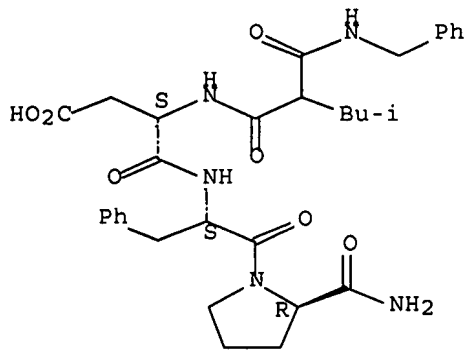
AB Peptidomimetics I (R1 = alkyl, aminoalkyl, or a ring structure which may form at R1, between R1 and R2 or between R1 and R4; R2 = H, Me or R2 and R1 form the R1 ring structure group; R3 = alkyl, alkyl alc., thioalkyl or a ring structure; R4 = H or R4 and R1 form the R1 ring structure; R5 = H or R5 and R6 form a ring structure; R6 = benzyl, 1,1-diphenylmethine, or the R5 ring structure) were prepared as inhibitors of the binding between the VLA-4 receptor and the fibronectin CS-1 domain. Thus, N-phenylacetyl-Leu-Asp-Phe-D-Pro-NH2 was prepared and assayed for binding inhibition potency (313 relative to a standard compound).

IT *209601-97-8P 209602-44-8P*
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of CS-1 peptidomimetics and their compns.)

RN 209601-97-8 CAPLUS

CN D-Prolinamide, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)-β-alanyl-L-α-aspartyl-L-phenylalanyl- (9CI) (CA INDEX NAME)

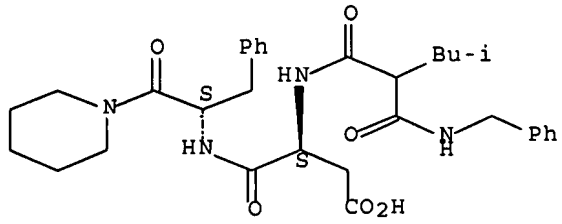
Absolute stereochemistry.



RN 209602-44-8 CAPLUS

CN L-α-Asparagine, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-2-oxo-1-(phenylmethyl)-2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 19 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:427769 CAPLUS Full-text

DOCUMENT NUMBER: 129:95722

TITLE: Preparation of CS-1 peptidomimetics and their compositions

INVENTOR(S): Arrhenius, Thomas S.; Elices, Mariano J.; Gaeta, Federico C. A.

PATENT ASSIGNEE(S): Cytel Corp., USA

SOURCE: U.S., 80 pp., Cont.-in-part of U.S. Ser. No. 349,024. CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

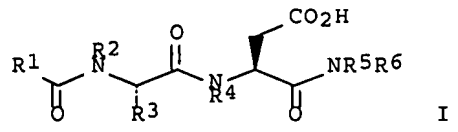
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5770573	A	19980623	US 1995-462219	19950605
CA 2177840	A1	19950615	CA 1994-2177840	19941205
CN 1142832	A	19970212	CN 1994-194969	19941205
US 5688913	A	19971118	US 1995-435286	19950505
US 6117840	A	20000912	US 1997-837154	19970414
US 6103870	A	20000815	US 1997-923026	19970903

PRIORITY APPLN. INFO.: US 1993-164101 B2 19931206
US 1994-349024 A2 19941202
US 1995-435286 A1 19950505

OTHER SOURCE(S): MARPAT 129:95722

GI



I

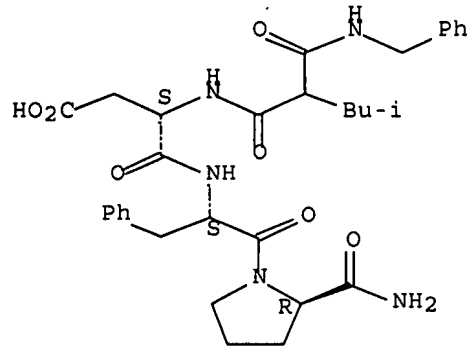
AB Peptidomimetics I (R1 = alkyl, aminoalkyl, or a ring structure which may form at R1, between R1 and R2 or between R1 and R4; R2 = H, Me or R2 and R1 form the R1 ring structure group; R3 = alkyl, alkyl alc., thioalkyl or a ring structure; R4 = H or R4 and R1 form the R1 ring structure; R5 = H or R5 and R6 form a ring structure; R6 = benzyl, 1,1-diphenylmethine, or the R5 ring structure) were prepared as inhibitors of the binding between the VLA-4 receptor and the fibronectin CS-1 domain. Thus, N-phenylacetyl-Leu-Asp-Phe-D-Pro-NH2 was prepared and assayed for binding inhibition potency (313 relative to a standard compound).

IT ***209601-97-8P 209602-44-8P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of CS-1 peptidomimetics and their compns.)

RN 209601-97-8 CAPLUS

CN D-Prolinamide, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)-β-alanyl-L-α-aspartyl-L-phenylalanyl- (9CI) (CA INDEX NAME)

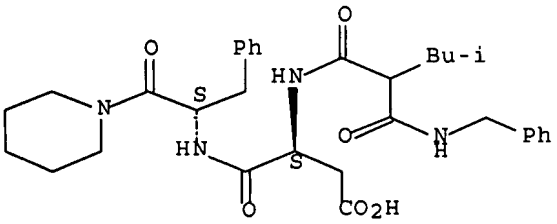
Absolute stereochemistry.



RN 209602-44-8 CAPLUS

CN L-α-Asparagine, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-2-oxo-1-(phenylmethyl)-2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

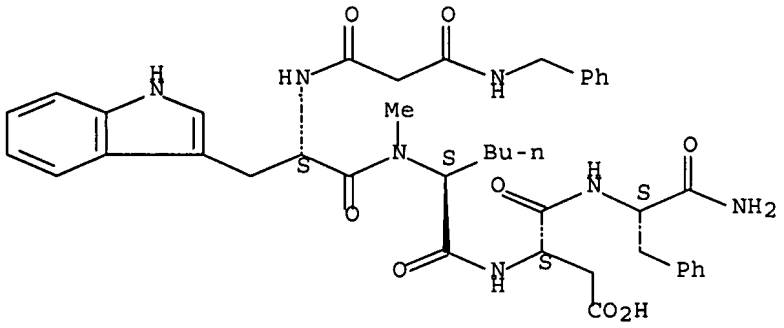
L53 ANSWER 20 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:82115 CAPLUS Full-text
DOCUMENT NUMBER: 128:188696
TITLE: Development of new potent agonists able to interact with two postulated subsites of the cholecystokinin CCK-B receptor
AUTHOR(S): Million, Marie-Emmanuelle; Lena, Isabelle; Da Nascimento, Sophie; Noble, Florence; Dauge, Valerie; Garbay, Christiane; Roques, Bernard Pierre
CORPORATE SOURCE: Dep. Pharmacochimie Moleculaire Structurale, Univ. Rene-Descartes-UFR Scis. Pharmaceutiques Biologiques, Paris, F-75270, Fr.
SOURCE: Letters in Peptide Science (1997), 4(4/5/6), 407-410
CODEN: LPSCEM; ISSN: 0929-5666
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Since the biochem. and pharmacol. profile of BC 197 and BC 264, two CCK8-derived agonists with high specificity for CCK-B receptors, suggests their potential interaction with two CCK-B receptor subsites, it appeared essential to design a new series of compds. that would be able to discriminate between these two subsites. As CCK4 is the shortest fragment of CCK which interacts selectively with CCK-B receptors, compds. derived from the C-terminal tetrapeptide domain of BC 264, Boc-Trp-(NMe)Nle-Asp- Phe-NH2, and of the cyclic compound BC 197, were prepared While RB 360 (N(cycloamido)-α-Me(R)Trp-[(2S)-2-amino-9- ((cycloamido)carbonyl)nonanoyl]-Asp-Phe-NH2), like BC 197, has a CCK-B1 profile with anxiogenic-like effects in the elevated plus-maze test, RB 400 (HOOC-CH2-CO-Trp-(NMe)Nle-Asp-Phe-NH2), like BC 264, seems to be a specific CCK-B2 agonist, able to increase attention and/or memory processes in the Y-maze test.

IT *203563-93-3*, RB 401
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(development of new potent agonists able to interact with two postulated subsites of cholecystokinin CCK-B receptor)

RN 203563-93-3 CAPLUS
CN L-Phenylalaninamide, 3-oxo-N-(phenylmethyl)-β-alanyl-L-tryptophyl-N-methyl-L-norleucyl-L-α-aspartyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 21 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:740382 CAPLUS Full-text
DOCUMENT NUMBER: 128:359
TITLE: Method for detecting and/or quantifying a hapten in a homogeneous phase using hapten-inhibitor complex, antibody, β-lactamase, and reporter substrate, and device for implementation thereof
INVENTOR(S): Kohl, Michel; Renotte, Roger; Ghitti, Gianangelo; Sarlet, Guy; Lejeune, Robert
PATENT ASSIGNEE(S): Biocode S.A., Belg.; Kohl, Michel; Renotte, Roger; Ghitti, Gianangelo; Sarlet, Guy; Lejeune, Robert
SOURCE: PCT Int. Appl., 67 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9741435	A1	19971106	WO 1997-BE52	19970430
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, DE, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
BE 1010184	A3	19980203	BE 1996-384	19960430
CA 2252931	A1	19971106	CA 1997-2252931	19970430
AU 9726286	A	19971119	AU 1997-26286	19970430
EP 897540	A1	19990224	EP 1997-917955	19970430
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
JP 2000509495	T	20000725	JP 1997-538408	19970430
AT 202848	T	20010715	AT 1997-917955	19970430
US 6436649	B1	20020820	US 1999-171819	19990611
US 2003235877	A1	20031225	US 2002-269673	20021010

PRIORITY APPLN. INFO.:		
BE 1996-384	A	19960430
WO 1997-BE52	W	19970430
US 1999-171819	A2	19990611
US 2002-75648	A1	20020213

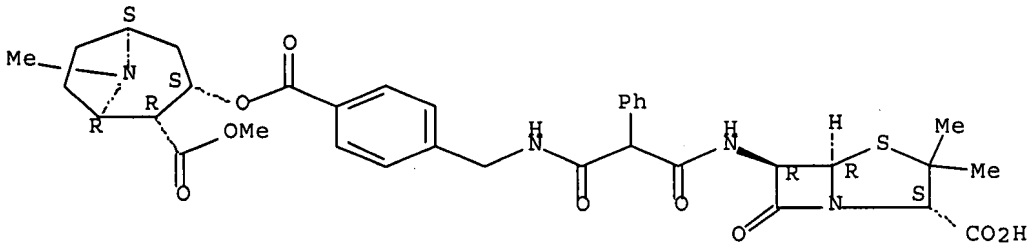
AB The invention discloses a method for detecting and/or quantifying a hapten (e.g. a drug or hormone) in a homogeneous phase, comprising the following steps: adding a known quantity of a hapten-inhibitor complex to the solution containing the hapten to be detected and/or quantified; adding to the solution a quantity of antibodies corresponding to the quantity of the hapten/inhibitor complex; adding to the solution a type C β-lactamase having an active site for two substrates in antigenic competition in the active site, the first substrate being a reporter substrate capable of being transformed into a detectable and/or quantifiable product, preferably by UV-visible radiation measurement, the second substrate being the hapten/inhibitor complex acting on the hydrolysis rate of the reporter substrate; detecting and/or quantifying the concentration of the product resulting from the transformation of the reporter substrate, the Km of the reporter substrate being at least a hundred times higher than the Km of the hapten/inhibitor complex, and the kcat being at least ten times higher than the kcat of the hapten/inhibitor complex. Preparation of reagent conjugates, e.g. nandrolone carbenicillinate, is described, as is determination of e.g. nandrolone.

IT *198830-23-8P*
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(hapten detection or determination in homogeneous phase using hapten-inhibitor
complex, antibody, β-lactamase, and reporter substrate, implementation device, and reagent preparation)

RN 198830-23-8 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[[4-[[[3-[[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]amino]-1,3-dioxo-2-phenylpropyl]amino]methyl]benzoyl]oxy]-8-methyl-, 2-methyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 22 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:481776 CAPLUS Full-text

DOCUMENT NUMBER: 127:217787

TITLE: Isolation and synthesis of rufulamide, an oligopeptide analog from Metzgeria rufula

AUTHOR(S): Kraut, Ludwig; Klaus, Thomas; Mues, Rudiger; Eicher, Theophil; Zinsmeister, Hans Dietmar

CORPORATE SOURCE: Fachbereich Botanik, Fachbereich Organische Chemie, Univ. Saarlandes, Saarbrucken, D-66041, Germany

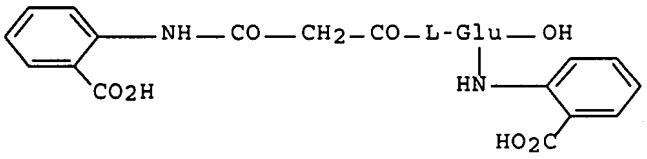
SOURCE: Phytochemistry (1997), 45(8), 1621-1626
CODEN: PYTCAS; ISSN: 0031-9422

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

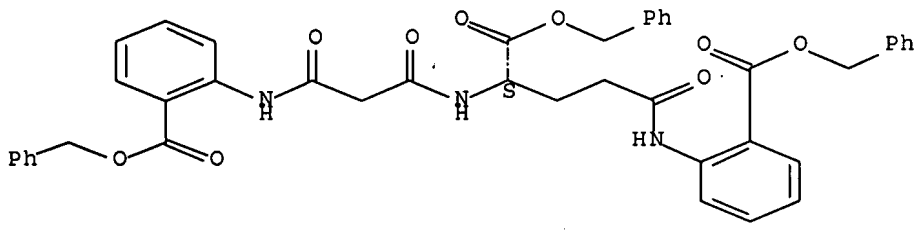
AB An oligopeptide analog, rufulamide (I), consisting of L-glutamic, malonic and 2 mols. of anthranilic acid combined via amide bonds was isolated from the liverwort Metzgeria rufula. Its structure was elucidated by spectroscopic methods and by chemical synthesis.

IT ***194875-99-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate in preparation of rufulamide)

RN 194875-99-5 CAPLUS

CN L-Glutamine, 3-oxo-N-[2-[(phenylmethoxy)carbonyl]phenyl]-β-alanyl-N-[2-[(phenylmethoxy)carbonyl]phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



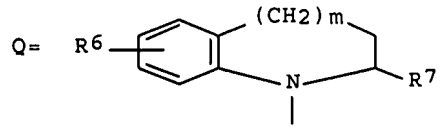
L53 ANSWER 23 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:462231 CAPLUS Full-text
DOCUMENT NUMBER: 125:115153
TITLE: Preparation of (acylamino)acetamide derivatives with agonist activity for cholecystokinin-A receptors
INVENTOR(S): Dezube, Milana; Hirst, Gavin Charles; Willson, Timothy Mark; Sherrill, Ronald George; Sugg, Elizabeth Ellen; Szewczyk, Jerzy Ryszard
PATENT ASSIGNEE(S): Glaxo Wellcome Inc., USA
SOURCE: PCT Int. Appl., 121 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9611940	A1	19960425	WO 1995-EP4026	19951012

W: AL, AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

AU 9538418	A	19960506	AU 1995-38418		19951012
EP 785944	A1	19970730	EP 1995-936483		19951012
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE					
JP 10511929	T	19981117	JP 1995-512935		19951012
US 5889182	A	19990330	US 1997-817363		19970414
PRIORITY APPLN. INFO.:			GB 1994-20763	A	19941014
			WO 1995-EP4026	W	19951012

OTHER SOURCE(S): MARPAT 125:115153
GI

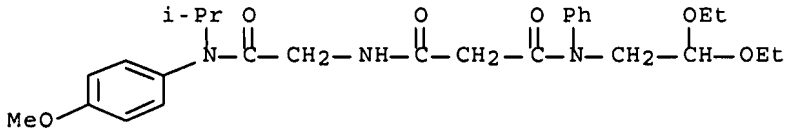


AB A cholecystokinin-A (CCK-A) agonist of the general formula R1R2NCOCH2NR3COR4 [R1 = C3-6 alkyl, C3-6 cycloalkyl, C3-6 alkenyl, Ph, (CH2)pCN, (CH2)pCO2(C1-4 alkyl); R2 = C3-6 alkyl, C3-6 cycloalkyl, C3-6 alkenyl, PhCH2, Ph or Ph mono- or disubstituted independently with C1-3 alkyl, CN, OH, NMe2, O(C1-4 alkyl), OCH2Ph, NH(C1-4 alkyl), CO2(C1-4 alkyl), N(C1-4 alkyl)2, pyrrolidino, morpholino, halo, C1-3 alkyl substituted by 1 or more F; R1 = C1-2 alkyl, R2 = 2- or 4-C6H4R, R = Cl, Me, MeO, CO2Me; R1R2N = Q; R3 = C1-6 alkyl; Ph or Ph substituted by 1 or 2 C1-3 alkyl, C1-4 alkoxy or halo groups, thiophenyl; R4 = CR6R9(CH2)n(NH)p(CO)q(NH)rR5, CH2N(CHR16R17)CO(NR)rR5; R5 = C1-6 alkyl, C3-8 cycloalkyl, Ph, mono- or disubstituted Ph, optionally substituted heteroaryl or bicycloheteroaryl; R6 = H, optionally substituted C1-3 alkyl; R7 = H, Me; R8 = H, OH, F, NMe2, C1-4 alkoxy, PhCH2O; R9 = H, C1-6 alkyl; R16 = C1-6 alkyl, C3-8 cycloalkyl, optionally halo substituted Ph, pyridyl, pyrimidinyl, thiophenyl; R17 together with R3 form o-disubstituted Ph ring optionally substituted with halo, CF3, C1-3 alkyl, C1-4 alkylthio, of C1-4 alkoxy; m = 0-2; n = 0-3; p = 0, 1; q = 0, 1; r = 0, 1] and physiol. acceptable salts thereof. Thus, ureidodipeptide amide PhNHCO-D-Glu-N(Ph)CH2CON(CHMe2)C6H4OMe-4, prepared in 4 steps from Boc-D-Glu(OCMe3)-OH, PhNH2, and BrCH2CON(CHMe2)C6H4OMe-4, was 55% as active as sulfated CCK-8 in a guinea pig gall bladder assay.

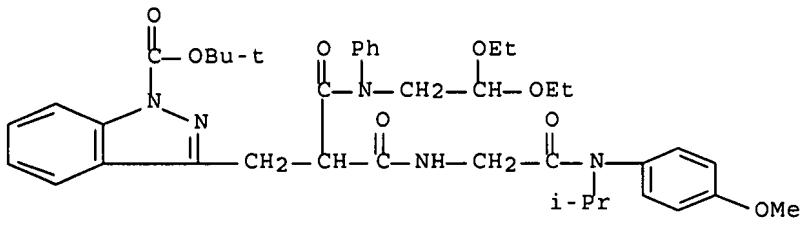
IT ***179083-73-9P 179083-74-0P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (acylamino)acetamide derivs. with agonist activity for cholecystokinin-A receptors)

RN 179083-73-9 CAPLUS

CN Glycinamide, N-(2,2-diethoxyethyl)-3-oxo-N-phenyl-β-alanyl-N-(4-methoxyphenyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 179083-74-0 CAPLUS
CN Glycinamide, N-(2,2-diethoxyethyl)-2-[[1-[(1,1-dimethylethoxy)carbonyl]-1H-indazol-3-yl]methyl]-3-oxo-N-phenyl-β-alanyl-N-(4-methoxyphenyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



L53 ANSWER 24 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:207549 CAPLUS Full-text
DOCUMENT NUMBER: 124:279362
TITLE: Inhibition of angiotensin converting enzyme and potentiation of bradykinin by retro-inverso analogs of short peptides and sequences related to angiotensin I and bradykinin
AUTHOR(S): Carmona, Adriana K.; Juliano, Luiz
CORPORATE SOURCE: Dep. Biophysics, Escola Paulista Medicina, Sao Paulo, Brazil
SOURCE: Biochemical Pharmacology (1996), 51(8), 1051-60
CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB There is pharmacol. evidence indicating that, in addition to the inhibition of angiotensin converting enzyme (ACE; EC 3.4.15.1), the potentiation of bradykinin (BK) responses may also involve the BK receptor or some binding site in the structures involved in the contractile response to this peptide. Dipeptides such as Val-Trp and some of its analogs as well as tripeptide homologs, including total and partial retro-inverso peptides, were synthesized and assayed for their ability to inhibit purified guinea pig plasma ACE and to potentiate the action of BK on the isolated ileum of the same species. The peptides containing the P2-P1, P1-P'1, and P'1-P'2 inverted amide bonds inhibited ACE, were resistant to hydrolysis, and, depending on the amino acid composition, some of them potentiated the contractile response to BK while others did not. Des-[Arg1]-BK, which has an intrinsic activity at concns. higher than 10-5M, and the very dissimilar angiotensin I (AI) analog [Cys5-Cys10]-angiotensin-I-(5-10)- amide, which has no detectable contractile activity, were able to inhibit ACE and potentiate BK. In contrast to these peptides, BPP5a and BPP9a from Bothrops jararaca venom, and potentiators B and C from Agkistrodon halys blomhoffi venom were more effective as BK potentiators than as ACE inhibitors. In conclusion, the authors have

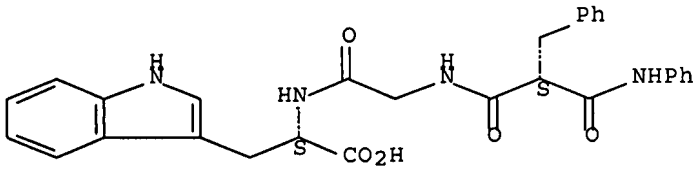
synthesized and assayed compds. that preferentially inhibit ACE, e.g. retro-inverso tripeptides, or potentiate the response of smooth muscle to BK, e.g. snake venom peptides.

IT *175412-96-1P*
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(angiotensin converting enzyme inhibition and bradykinin potentiation by angiotensin I and bradykinin short peptide retro-inverso analogs)

RN 175412-96-1 CAPLUS

CN L-Tryptophan, N-[N-[3-oxo-N-phenyl-(S)-2-(phenylmethyl)-β-alanyl]glycyl]- (9CI) (CA INDEX NAME)

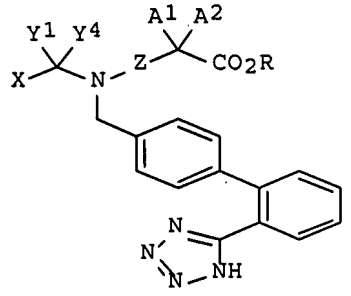
Absolute stereochemistry.



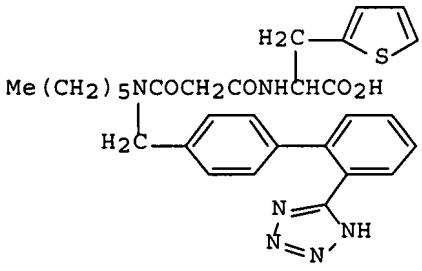
L53 ANSWER 25 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:828305 CAPLUS Full-text
DOCUMENT NUMBER: 123:228915
TITLE: Preparation of biphenylyltetrazole-containing amino acid and dipeptide derivatives as angiotensin II antagonists
INVENTOR(S): Naka, Yoichi; Sonda, Shuji; Nakagawa, Haruto; Uehata, Masayoshi
PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07048360	A	19950221	JP 1994-116464	19940530
PRIORITY APPLN. INFO.:			JP 1994-116464 A	19940530
			JP 1993-154348	19930531

OTHER SOURCE(S): MARPAT 123:228915
GI



I



II

AB The title compds. [I; X = (un)substituted NH2, alkenyl, cycloalkyl, aryl, or heteroaryl, saturated carbocyclyl containing NR in the ring; wherein R = H, acyl, alkoxycarbonyl, aralkoxycarbonyl; Y1, Y2 = H, alkyl, alkenyl, cycloalkyl, halo, OR1, NHR1, CO2 R1, CONHR1, COR1, aryl, heteroaryl; or Y1Y2 = O, S; wherein R1 = H, alkyl, alkenyl, cycloalkyl, aryl, heteroaryl; Z = CONH, CH2CONH, COCH2NH, COCH2CONH, single bond; when Z = CONH, A1A2 = cycloalkane ring optionally having a benzene ring-fused C5-7 substituent; when Z = CH2CONH, COCH2NH, COCH2CONH, or single bond, A1, A2 = H, (un)substituted alkyl, alkenyl, cycloalkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl or A1A2 = cycloalkane ring optionally having a benzene ring-fused C5-7 substituent], useful for the treatment of hypertension, ischemic heart failure, stroke, kidney diseases, and hypertrophy of the heart or blood vessels, are prepared Thus, H-Phe-OCH2Ph was alkylated by [2'-(triphenylmethyl-1H-tetrazol-5-yl)biphenyl-4-yl]methyl bromide in the presence of K2CO3 in DMF at room temperature for 24 h and then condensed with Z-Pro-Cl in aqueous NaHCO3/CH2Cl2 at room temperature for 3 h followed by deprotection with 2 N HCl/dioxane and hydrogenolysis over 10% Pd-C in EtOH-dioxane to give N-(S)-prolyl-N-[2'-(1H-tetrazol-5-yl)biphenyl-4- yl]methyl-(S)-phenylalanine. (RS)-(2-thienyl)alanine derivative (II) in vitro showed IC50 of 13 nM against angiotensin II in vascular smooth muscle cells of rat thoracic aorta.

IT ***168466-38-4P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

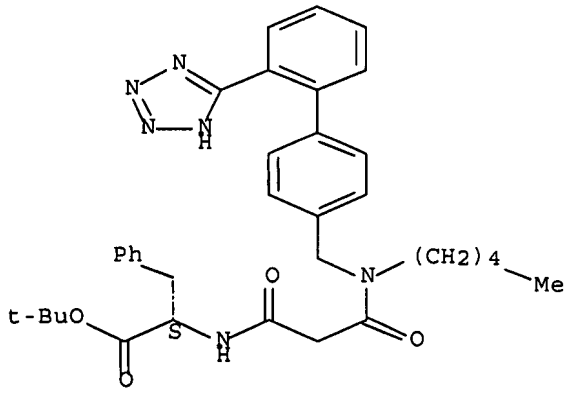
(intermediate for preparation of biphenylyltetrazole-containing amino acid and

dipeptide derivs. as angiotensin II antagonists)

RN 168466-38-4 CAPLUS

CN L-Phenylalanine, N-[3-oxo-N-pentyl-N-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-β-alanyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



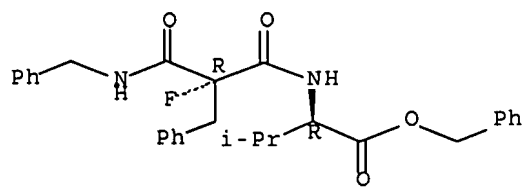
L53 ANSWER 26 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:643894 CAPLUS Full-text
DOCUMENT NUMBER: 123:313504
TITLE: New applications of fluorinated building blocks
AUTHOR(S): Abouabdellah, A.; Boros, L.; Gyenes, F.; Welch, J. T.
CORPORATE SOURCE: Department of Chemistry, State University of New York, Albany, NY, 12222, USA
SOURCE: Journal of Fluorine Chemistry (1995), 72(2), 255-9
CODEN: JFLCAR; ISSN: 0022-1139
PUBLISHER: Elsevier Sequoia
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:313504

AB A new and versatile synthesis of optically active α-fluoromalonamide derivs. from enantiomerically pure 3-fluoro-2-azetidinones is described. A fluorinated retroamide isostere based on these α-fluoromalonamides was introduced into a small peptidomimetic for use as an HIV-1 protease inhibitor. The same strategy was employed in efforts to prepare a novel trifluorostatone-type peptidomimetic.

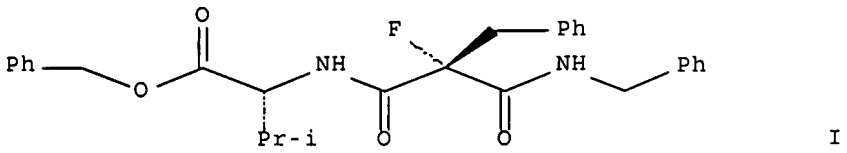
IT ***160000-01-1P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(versatile synthesis of optically active α-fluoromalonamide derivs. from enantiomerically pure 3-fluoro-2-azetidinones)

RN 160000-01-1 CAPLUS
CN D-Valine, N-[2-fluoro-1,3-dioxo-2-(phenylmethyl)-3-[(phenylmethyl)amino]propyl]-, phenylmethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 27 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:30147 CAPLUS Full-text
DOCUMENT NUMBER: 122:56436
TITLE: Optically active fluorinated β-lactam building blocks: a novel fluorinated retroamide isostere
AUTHOR(S): Abouabdellah, Ahmed; Welch, John T.
CORPORATE SOURCE: Department of Chemistry, State Univ. New York, Albany, NY, 12222, USA
SOURCE: Tetrahedron: Asymmetry (1994), 5(6), 1005-13
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

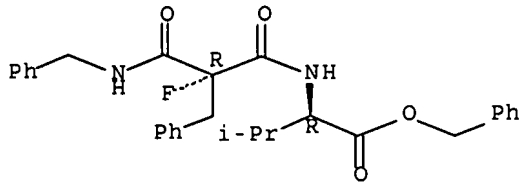
AB A new and versatile synthesis of optically active α-fluoro- malonamide derivs. from enantiomerically pure 3-fluoro-2-azetidinones is described. A fluorinated retroamide isostere, (-)-(R)- HO2CCF(CH2Ph)CONHCH2Ph, was introduced into a small peptidomimetic(I) for use as an HIV-1 protease inhibitor.

IT ***160000-01-1P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of valylfluoromalonamides)

RN 160000-01-1 CAPLUS

CN D-Valine, N-[2-fluoro-1,3-dioxo-2-(phenylmethyl)-3-[(phenylmethyl)amino]propyl]-, phenylmethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

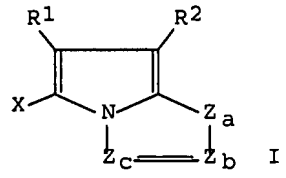


L53 ANSWER 28 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:641574 CAPLUS Full-text
DOCUMENT NUMBER: 121:241574
TITLE: Silver halide color photographic photosensitive material
INVENTOR(S): Nakagawa, Hajime; Shimada, Yasuhiro
PATENT ASSIGNEE(S): Fuji Photo Film Co Ltd, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 73 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05297538	A	19931112	JP 1992-121080	19920416
PRIORITY APPLN. INFO.:			JP 1992-121080	19920416

GI



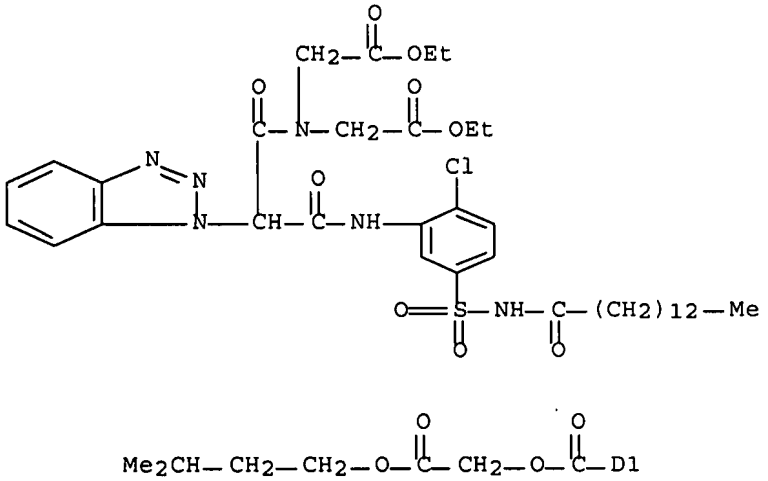
I

AB The title material contains ≥1 kind(s) of cyan couplers I (Za = NH, CHR3; Zb, Zc = CR4, N; R1-3 = electron-withdrawing group having a Hammett's substituent constant σp >0.20; the sum of the σp values of R1 and R2 is >0.65; R4 = H, substrate, if there are >2 of R4 they may be the same or different; X = H, group to be eliminated upon coupling; R1-4 or X may become a divalent group and bond with a polymer which is larger than a dimer or a polymer chain to form a homopolymer or a copolymer) and ≥1 kind(s) of development inhibitor-releasing couplers A-{(L1)a-(B)m}p-(L2)n-DI [A = group which splits {(L1)a-(B)m}p-(L2)n-DI upon reaction with an oxidized aromatic primary amine developing agent; L1 = group which splits the bond at its right side (the bond with (B)n) after breaking the bond at its left side; B = group which splits the bond at its right side upon reaction with an oxidized developing agent; L2 = group which splits the bond at its right side (the bond with DI) after breaking the bond at its left side; DI = development inhibitor; a, m, n = 0, 1; p = 0-2, when p is plural (L1)a-(B)m may be the same or different]. The material shows good color reproducibility and superior shelf life.

IT ***158372-17-9***
RL: USES (Uses)
(photog. development inhibitor-releasing coupler)

RN 158372-17-9 CAPLUS

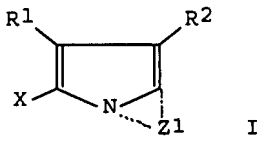
CN 1H-Benzotriazolecarboxylic acid, 1-[1-[[bis(2-ethoxy-2-oxoethyl)amino]carbonyl]-2-[[2-chloro-5-[[(1-oxotetradecyl)amino]sulfonyl]phenyl]amino]-2-oxoethyl]-, 2-(3-methylbutoxy)-2-oxoethyl ester (9CI) (CA INDEX NAME)



L53 ANSWER 29 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:495837 CAPLUS Full-text
DOCUMENT NUMBER: 121:95837
TITLE: Silver halide color photographic materials with excellent color reproducibility and storage stability
INVENTOR(S): Nakagawa, Hajime; Yamakawa, Kazuyoshi
PATENT ASSIGNEE(S): Fuji Photo Film Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 75 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05281680	A	19931029	JP 1992-108460	19920402
PRIORITY APPLN. INFO.:			JP 1992-108460	19920402

GI



I

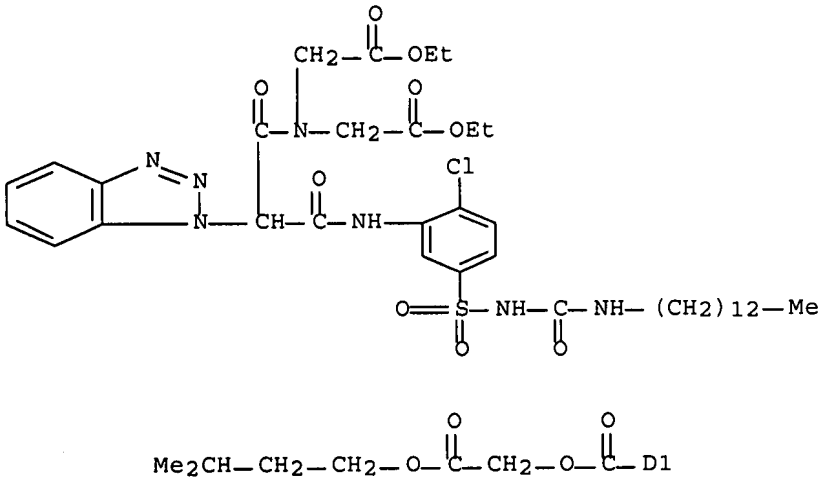
AB The Ag halide color photog. material, comprising ≥1 red-, green-, and blue-sensitive Ag halide emulsion layers on a support, contains a cyan coupler I [R1 = H, substituent; R2 = substituent; X = H, moiety released upon coupling reaction with oxidation products of color developing agent; Z1 = nonmetallic atomic group forming N-containing 6-membered heterocyclyl; heterocyclyl contains ≥1 dissociating moiety] and a DIR coupler A-{(L1)a-(B)n}p-(L2)n-DI [A

= moiety releasing {(L1)a-(B)n}p-(L2)n-DI upon reacting with aromatic primary amine developing agent; L1 = moiety released from A and then from B; B = moiety released from L2 upon reaction with oxidation products of developing agent; L2 = moiety relased from C and then from DI; DI = development inhibitor; a, m, n = 0, 1; p = 0-2].

IT *156343-04-3*
RL: USES (Uses)
(silver halide color photog. material containing)

RN 156343-04-3 CAPLUS

CN 1H-Benzotriazolecarboxylic acid, 1-[1-[[bis(2-ethoxy-2-oxoethyl)amino]carbonyl]-2-[[2-chloro-5-[[[(tridecylamino)carbonyl]amino]sulfonyl]phenyl]amino]-2-oxoethyl]-, 2-(3-methylbutoxy)-2-oxoethyl ester (9CI) (CA INDEX NAME)



L53 ANSWER 30 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:482789 CAPLUS Full-text

DOCUMENT NUMBER: 121:82789

TITLE: Acid-aided reactions of 3-acylamino-β-lactams: some observations

AUTHOR(S): Sanjayan, Gangadhar J.; Mukerjee, Arya K.

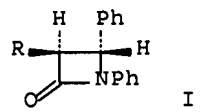
CORPORATE SOURCE: Fac. Sci., Banaras Hindu Univ., Varanasi, 221 005, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1994), 33B(1), 76-8
CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

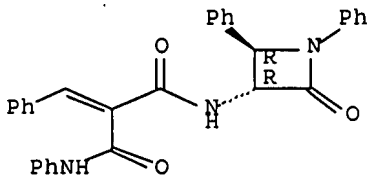
AB 3-Benzoylamino-1,4-diphenylazetidin-2-one (I, R = BzNH) gives 2-benzoylaminocinnamanilide and 4-benzylidene-1,2-diphenylimidazolin-5-one when heated in gl. acetic acid containing concentrated H_2SO_4. I (R = AcNH) forms tar under similar conditions, but in the presence of benzaldehyde it affords 2-cinnamoylaminocinnamanilide and 4-benzylidene-2-styryl-2- imidazolin-5-one. I [R = PhCH:C(NHBz)CONH], on the other hand furnishes 4-benzylidene-2-phenyl-2-oxazolin-5-one and 3-amino-1,4-diphenylazetidin-2- one. Mechanisms are given.

IT ***156486-82-7***
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acids)

RN 156486-82-7 CAPLUS

CN Propanediamide, N-(2-oxo-1,4-diphenyl-3-azetidinyl)-N'-phenyl-2-(phenylmethylene)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



L53 ANSWER 31 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:446485 CAPLUS Full-text
DOCUMENT NUMBER: 121:46485
TITLE: Silver halide color photographic materials
INVENTOR(S): Saito, Naoki; Ogawa, Akira; Nakagawa, Hajime
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 58 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 568037	A1	19931103	EP 1993-106891		19930428
EP 568037	B1	19981104			
R: BE, DE, FR, GB, NL					
JP 05307248	A	19931119	JP 1992-134523		19920428
JP 2835665	B2	19981214			
US 5459024	A	19951017	US 1995-400269		19950303
PRIORITY APPLN. INFO.:			JP 1992-134523	A	19920428
			US 1993-52670	B1	19930427

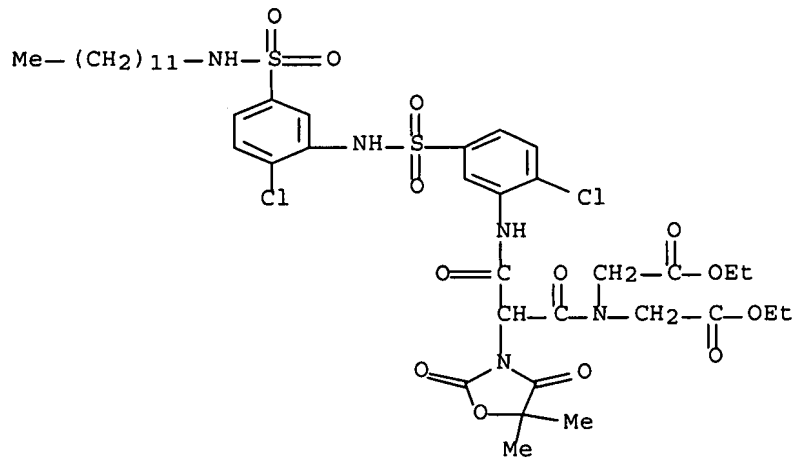
OTHER SOURCE(S): MARPAT 121:46485

AB The present invention relates to silver halide color photog. materials having improved sharpness, higher photog. speeds and increased fastness by forming images in the presence of couplers wherein the rate of dye formation is high, the color forming d. is high and the dye which is formed has a high degree of fastness. A photog. coupler represented by the formula R1R2NCOCHXCONHZSO2NR3R4 wherein R1 and R2 each independently represents an alkyl group, an aryl group or a heterocyclic group, R3 represents a hydrogen atom, an alkyl group, an aryl group or a heterocyclic group, X represents a group which can be eliminated when the coupler reacts with an oxidized product of a primary aromatic amine developing agent, Z represents a phenylene group, R4 represents an aryl group or a heterocyclic group, and R1 and R2, R3 and Z, or R3 and R4 may be linked to form a ring is contained in at least one hydrophilic colloid layer of the silver halide color photog. materials.

IT ***155926-64-0***
RL: TEM (Technical or engineered material use); USES (Uses)
(photog. coupler)

RN 155926-64-0 CAPLUS

CN Glycine, N-[N-[2-chloro-5-[[[2-chloro-5-[(dodecylamino)sulfonyl]phenyl]amino]sulfonyl]phenyl]-2-(5,5-dimethyl-2,4-dioxo-3-oxazolidinyl)-3-oxo-β-alanyl]-N-(2-ethoxy-2-oxoethyl)-, ethyl ester (9CI) (CA INDEX NAME)



L53 ANSWER 32 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	1993:539079 CAPLUS Full-text
DOCUMENT NUMBER:	119:139079
TITLE:	Preparation of (pyrrolidinoethyl)urea derivatives as analgesics
INVENTOR(S):	Takeuchi, Makoto; Takayama, Kazuhisa; Onda, Kenichi; Motoie, Hiroyuki; Isomura, Yasuo
PATENT ASSIGNEE(S):	Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE:	PCT Int. Appl., 93 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	Japanese
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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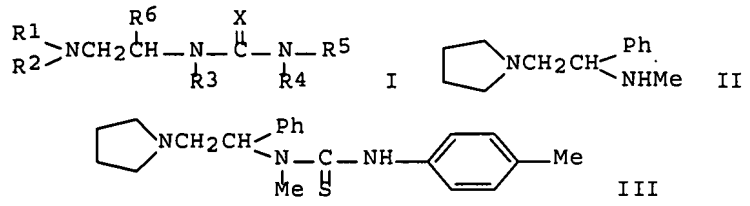
WO 9303011	A1	19930218	WO 1992-JP993		19920804
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, US					
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG					
AU 9223908	A	19930302	AU 1992-23908		19920804
CN 1069490	A	19930303	CN 1992-109284		19920807
PRIORITY APPLN. INFO.:			JP 1991-223280	A	19910808
			JP 1991-309952	A	19911029
			WO 1992-JP993	A	19920804

OTHER SOURCE(S): MARPAT 119:139079

GI



I II III

AB The title compds. [I; R1, R2 = alkyl, alkenyl, alkynyl, cycloalkyl, R1R2N pyrrolidino; R3, R4 = H, alkyl, alkenyl, alkynyl, cycloalkyl; R3R4 = alkylene, alkenylene, etc.; R5 = (substituted) carbocyclic, condensed heterocyclyl containing 1 or 2 O and/or S atoms; R6 = (substituted) Ph; X = O, S] are prepared A mixture of 4-MeC6H4NCS and pyrrolidine derivative (S)-II in ClCH2CH2Cl was stirred at room temperature to give thiourea (S)-III, which was treated with 4N HCl in EtOAc to give (S)-III.HCl. III.HCl showed EO50 of 0.54 mg/kg s.c. in mice in the tail pinch test. Tablet, capsule, injection formulations were given.

IT ***149865-92-9P***

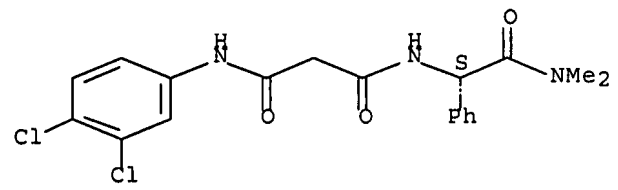
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of analgesics)

RN 149865-92-9 CAPLUS

CN Propanediamide, N-(3,4-dichlorophenyl)-N'-[2-(dimethylamino)-2-oxo-1-phenylethyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

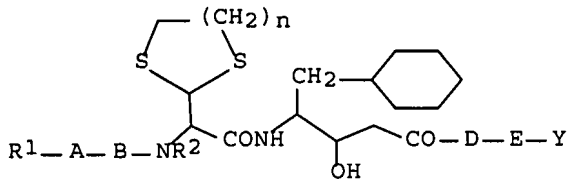


L53 ANSWER 33 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

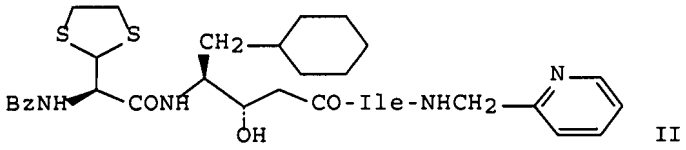
ACCESSION NUMBER: 1992:612973 CAPLUS Full-text
DOCUMENT NUMBER: 117:212973
TITLE: Renin-inhibiting peptides of the cyclohexylstatine type
INVENTOR(S): Bender, Wolfgang; Schmidt, Gunter; Knorr, Andreas; Stasch, Johannes Peter
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 61 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4038921	A1	19920611	DE 1990-4038921	19901206
WO 9210509	A1	19920625	WO 1991-EP2300	19911203
W: AU, BG, BR, CA, CS, FI, HU, JP, KR, NO, PL, RO, SU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
AU 9190252	A	19920708	AU 1991-90252	19911203
JP 06503315	T	19940414	JP 1992-500344	19911203
PRIORITY APPLN. INFO.:			DE 1990-4038921 A	19901206
			WO 1991-EP2300 A	19911203

OTHER SOURCE(S): MARPAT 117:212973
GI



I



II

AB Peptides I [A, B, D, E = bond, (un)protected amino acid; R1 = H, protective group, acyl; R2 = H, alkyl, CH2Ph; R1-A-B-NR2 = heterocyclic; Y = H, alkyl, cycloalkyl, protective group) (un)substituted NH2; n = 1, 2] were prepared as plasma renin inhibitors (no data). Thus, peptide II was obtained from amino(dithiolene)acetic acid in 4 steps.

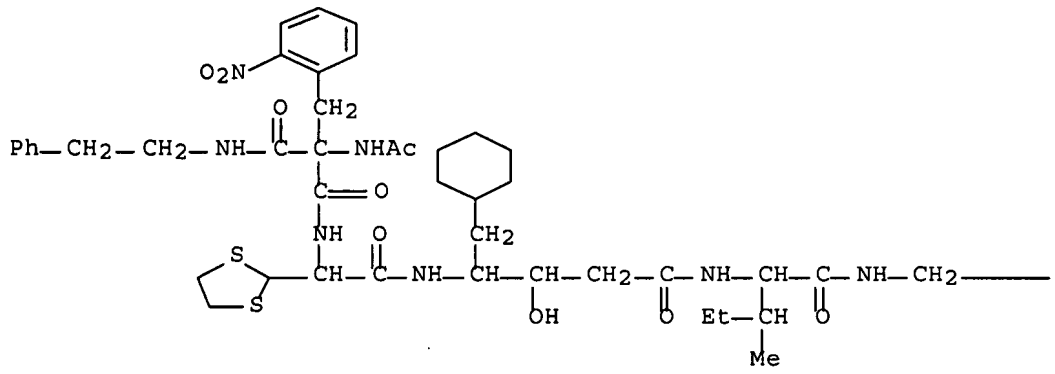
IT ***144165-68-4P 144299-10-5P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 144165-68-4 CAPLUS

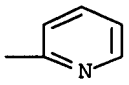
CN L-threo-Pentonamide, 4-[[N-[N-acetyl-2-nitro-α-[[(2-phenylethyl)amino]carbonyl]-D-phenylalanyl]-L-2-(1,3-dithiolan-2-yl)glycyl]amino]-5-cyclohexyl-2,4,5-trideoxy-N-[2-methyl-1-[[(2-

pyridinylmethyl)amino]carbonyl]butyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

PAGE 1-A



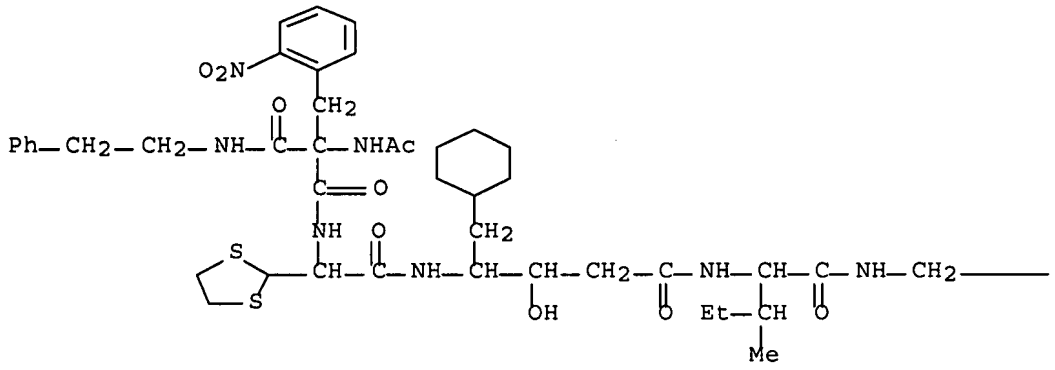
PAGE 1-B



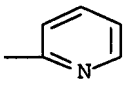
RN 144299-10-5 CAPLUS

CN L-threo-Pentonamide, 4-[[N-[N-acetyl-2-nitro-α-[[(2-phenylethyl)amino]carbonyl]-L-phenylalanyl]-L-2-(1,3-dithiolan-2-yl)glycyl]amino]-5-cyclohexyl-2,4,5-trideoxy-N-[2-methyl-1-[[(2-pyridinylmethyl)amino]carbonyl]butyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



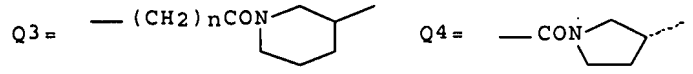
L53 ANSWER 34 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:129634 CAPLUS Full-text
DOCUMENT NUMBER: 116:129634
TITLE: Preparation of amidino derivatives of peptides and amino acids as drugs
INVENTOR(S): Alig, Leo; Edenhofer, Albrecht; Mueller, Marcel; Trzeciak, Arnold; Weller, Thomas
PATENT ASSIGNEE(S): Hoffmann-La Roche, F., A.-G., Switz.
SOURCE: Eur. Pat. Appl., 28 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 445796	A2	19910911	EP 1991-103462	19910307
EP 445796	A3	19911030		
EP 445796	B1	19980617		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
CA 2037153	A1	19910910	CA 1991-2037153	19910226

ZA 9101534	A	19911127	ZA 1991-1534		19910301
HU 56582	A2	19910930	HU 1991-186		19910304
AU 9172086	A	19920820	AU 1991-72086		19910304
AU 646838	B2	19940310			
IL 97401	A	19950315	IL 1991-97401		19910304
US 5273982	A	19931228	US 1991-665110		19910305
FI 9101148	A	19910910	FI 1991-1148		19910307
JP 04217652	A	19920807	JP 1991-65316		19910307
JP 2501252	B2	19960529			
RU 2072359	C1	19970127	RU 1991-4894657		19910307
AT 167482	T	19980715	AT 1991-103462		19910307
ES 2118067	T3	19980916	ES 1991-103462		19910307
NO 9100934	A	19910910	NO 1991-934		19910308
NO 301167	B1	19970922			
BR 9100941	A	19911105	BR 1991-941		19910308
PRIORITY APPLN. INFO.:			CH 1990-775	A	19900309
			CH 1991-115	A	19910117
			CH 1991-192		19910123

OTHER SOURCE(S): MARPAT 116:129634

GI



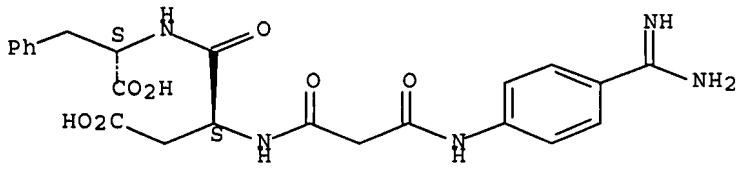
AB H2N(HN:)C-X-Y-CO-Z-CH(Q1)CO2Q2 [Q1 = H, Me, Ph; Q2 = H, phenylalkyl, physiol. cleavable alkyl; X = phenylene, pyridylene, piperidinylene; Y = CH2CH2NHCOCH2, NHCO(CH2)3, Q3, Q4, etc.; n = 0-2; Z = piperazinylene, piperidinylene, NHCH2, NHCHMe, etc.], were prepared Thus, H-β-Ala-Asp(OCMe3)-Phe-OCMe3 (preparation given) was condensed with 4-NCC6H4CO2H to give the N-cyanobenzoyl derivative, which was treated with H2S in pyridine/Et3N to give the N-thiocarbamoylbenzoyl derivative The latter was refluxed with MeI in acetone and the product was refluxed with NH4OAc in MeOH to give the protected N-amidinobenzoyl derivative, which was treated with CF3CO2H to give N-[N-[N-(p-amidinobenzoyl)-β-alanyl]-α- aspartyl]-3-phenylalanine trifluoroacetate. The latter inhibited fibrinogen binding to its receptor (glycoprotein IIb/IIIa) with IC50 = 0.003 μM.

IT *138107-62-7P 138108-00-6P*
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as drug)

RN 138107-62-7 CAPLUS

CN L-Phenylalanine, N-[N-[N-[4-(aminoiminomethyl)phenyl]-3-oxo-β-alanyl]-L-α-aspartyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

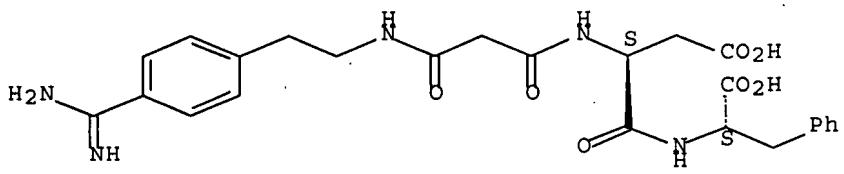


RN 138108-00-6 CAPLUS
CN L-Phenylalanine, N-[N-[N-[2-[4-(aminoiminomethyl)phenyl]ethyl]-3-oxo-β-alanyl]-L-α-aspartyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

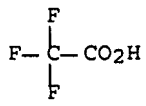
CRN 138107-99-0
CMF C25 H29 N5 O7

Absolute stereochemistry.



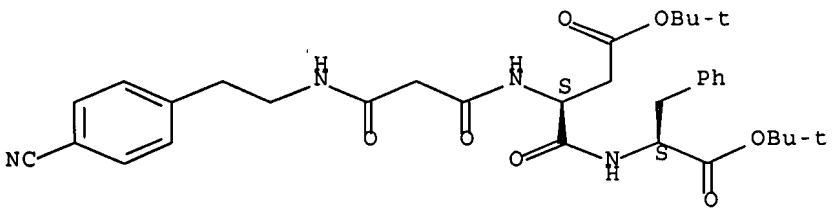
CM 2

CRN 76-05-1
CMF C2 H F3 O2



IT *138135-00-9P*
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as drug intermediate)
RN 138135-00-9 CAPLUS
CN L-Phenylalanine, N-[N-[N-[2-(4-cyanophenyl)ethyl]-3-oxo-β-alanyl]-L-α-aspartyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

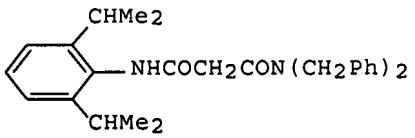
Absolute stereochemistry.



L53 ANSWER 35 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:655831 CAPLUS Full-text
DOCUMENT NUMBER: 115:255831
TITLE: Preparation of N,N'-disubstituted malonamides as cholesterol acyltransferase inhibitors
INVENTOR(S): Roark, William H.
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: Can. Pat. Appl., 50 pp.
CODEN: CPXXEB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2030105	A1	19910517	CA 1990-2030105	19901115
AU 9066590	A	19910613	AU 1990-66590	19901113
FI 9005645	A	19910517	FI 1990-5645	19901114
NO 9004955	A	19910521	NO 1990-4955	19901115
EP 433662	A2	19910626	EP 1990-121904	19901115
EP 433662	A3	19910703		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU 57705	A2	19911230	HU 1990-7154	19901115
ZA 9009186	A	19920729	ZA 1990-9186	19901115
CN 1051733	A	19910529	CN 1990-109182	19901116
JP 03220164	A	19910927	JP 1990-308982	19901116
PRIORITY APPLN. INFO.:			US 1989-437727 A	19891116
			US 1990-594484 A	19901009

OTHER SOURCE(S): MARPAT 115:255831
GI



I

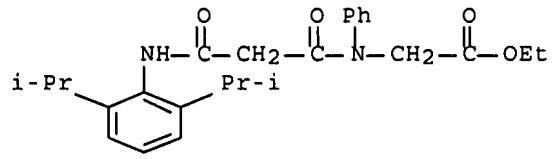
AB Title compds. ArNHCO(CH2)mCR3R4(CH2)nCONR1R2 [Ar = (CH2)xR; (substituted) naphthyl; R = (substituted) Ph; m, n, x = 0-2; R3, R4 = H, (hydroxy)C1-10 alkyl, (amino)C1-10 alkyl; 1 of R3, R4 = H and the other = amino; R1, R2 = H, (CH2)tCR7R8(CH2)wR9, C1-20 hydrocarbyl, (amino)C1-6 alkyl, (carboalkoxy)C1-6

alkyl, (substituted) Ph, etc.; R7, R8 = H, C1-6 alkyl; R9 = (substituted) Ph or R8 = (substituted) Ph when R7 = H; t, w = 0-4; t + w ≤ 5] were prepared as cholesterol acyltransferase inhibitors. Thus, 2,6-diisopropylaniline was condensed with ClCOCH2CO2Et and the product was hydrolyzed to carboxymethyl amide. This was coupled with (PhCH2)2NH to give title compound I. I had IC50 of 0.013 μM against cholesterol acyltransferase. I lowered blood cholesterol by 42 mg/dL in rats.

IT *137379-32-9P*
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as cholesterol acyltransferase inhibitor)

RN 137379-32-9 CAPLUS

CN Glycine, N-[3-[[2,6-bis(1-methylethyl)phenyl]amino]-1,3-dioxopropyl]-N-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



L53 ANSWER 36 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:123053 CAPLUS Full-text

DOCUMENT NUMBER: 114:123053

TITLE: Synthesis of human renin inhibitory peptides, angiotensinogen transition-state analogs containing a retro-inverso amide bond

AUTHOR(S): Harada, Hiromu; Iizuka, Kinji; Kamijo, Tetsuhide; Akahane, Kenji; Yamamoto, Ryoji; Nakano, Yasushi; Tsubaki, Atsushi; Kubota, Tetsuhiro; Shimaoka, Iwao; et al.

CORPORATE SOURCE: Cent. Res. Lab., Kissei Pharm. Co., Ltd., Matsumoto, 399, Japan

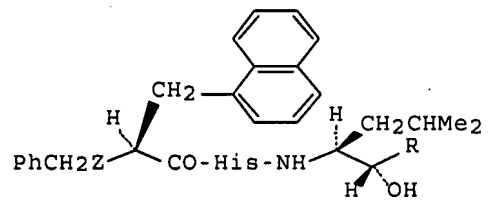
SOURCE: Chemical & Pharmaceutical Bulletin (1990), 38(11), 3042-7
CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:123053

GI



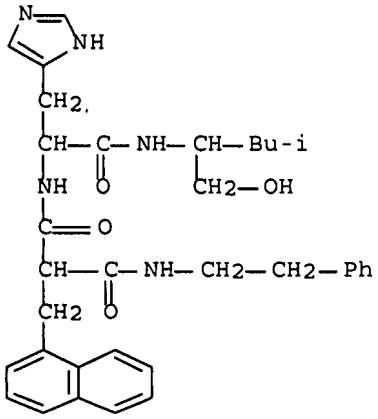
I

AB The exptl. details for the synthesis of human renin inhibitors I (Z = CH2NHCOCH2, R = H, CONHCH2CH2CHMe2, CO2Me, CH2CO2Me; Z = O2CNH, CONHCH2, CH2NHCO, NHCOCH2, R = H) are described. In order to avoid metabolic degradation of the Phe-His amide bond in transition-state analogs, structurally modified acyl residues were incorporated into the inhibitors. I (Z = CH2NHCOCH2, R = CONHCH2CH2CMe2) had potent human renin inhibitory activity, and it lowered blood pressure when administered orally to common marmosets.

IT ***132413-89-9P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and renin inhibitory activity of)

RN 132413-89-9 CAPLUS

CN Propanediamide, N-[2-[[1-(hydroxymethyl)-3-methylbutyl]amino]-1-(1H-imidazol-4-ylmethyl)-2-oxoethyl]-2-(1-naphthalenylmethyl)-N'-(2-phenylethyl)-, [2S-[1[R*(R*)],2R*]]- (9CI) (CA INDEX NAME)



L53 ANSWER 37 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1990:526032 CAPLUS Full-text

DOCUMENT NUMBER: 113:126032

TITLE: The anti-leishmanial activity of dipeptide esters on Leishmania amazonensis amastigotes

AUTHOR(S): Ramazeilles, C.; Juliano, L.; Chagas, J. R.; Rabinovitch, M.

CORPORATE SOURCE: Unite Immunoparasitol., Inst. Pasteur, Paris, 75724, Fr.

SOURCE: Parasitology (1990), 100(2), 201-7
CODEN: PARAAE; ISSN: 0031-1820

DOCUMENT TYPE: Journal

LANGUAGE: English

AB L-Amino acid esters, such as L-Leu-OMe, kill L. amazonensis amastigotes by a mechanism which appears to involve ester hydrolysis by cysteine proteinases located in the parasite megasomes. The killing of isolated amastigotes by L-dipeptide esters and some structure-activity correlations were demonstrated. Toxicity of the compds. for the parasites was measured by a tetrazolium (MTT) reduction assay. The results show that active dipeptide esters contained at least 1 hydrophobic amino acid (Leu, Ile, Val, Phe or Trp). The activity of

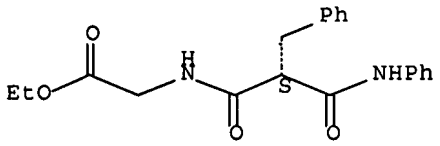
homodipeptide Me esters depended on the nature of the amino acid, as indicated by the following series: Phe-Phe-OMe > Val-Val-OMe > Leu-Leu-OMe > Trp-Trp-OMe > Ile-Ile-OMe. The nature of the amino acids in Leu-X-OMe and X-Leu-OMe was relatively unimportant when X was Phe, Trp or Val. However, when X was Ala or Gly, Leu-X-OMe was several-fold more active than X-Leu-OMe. A similar preference for the more hydrophobic residue in the amino terminal position was also found in esters containing a single phenylalanine or valine. Protection of the amino group by benzyloxycarbonyl (Z) or t-butyloxycarbonyl (BOC) substituents markedly enhanced the activity of the esters. An-mPhe-Gly-OEt, a retro-inverso analog of Bz-Phe-Gly-OEt, was several-fold more active than the parent compound Selected esters were assayed on infected macrophages and concns. that induced minimal toxicity to the host cells were estimated The ED50s for intracellular parasites were 1.5 to 5-fold higher than those for isolated amastigotes. Therapeutic ratios (concentration for detectable toxicity for macrophages/ED90) ranged from 1.6 (for Z-Leu-Gly-OMe) to 8 (for Val-Val-OMe).

IT *129279-73-8*
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antileishmanial activity of, on Leishmania amazonensis amastigotes, structure in relation to)

RN 129279-73-8 CAPLUS

CN Glycine, N-[1,3-dioxo-3-(phenylamino)-2-(phenylmethyl)propyl]-, ethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



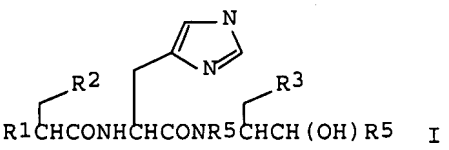
L53 ANSWER 38 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989:154893 CAPLUS Full-text
DOCUMENT NUMBER: 110:154893
TITLE: Preparation and testing of arylalanylhistidineamides as renin inhibitors
INVENTOR(S): Nakano, Kohji; Fujikura, Takashi; Hara, Ryuichiro; Ichihara, Masato; Fukunaga, Yikiko; Shibasaki, Masayuki
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 48 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 281316	A2	19880907	EP 1988-301609	19880225
EP 281316	A3	19900816		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FI 8800734	A	19880828	FI 1988-734	19880217
FI 89058	B	19930430		

FI 89058	C	19930810			
US 4904660	A	19900227	US 1988-160173		19880225
NO 8800851	A	19880829	NO 1988-851		19880226
JP 02009865	A	19900112	JP 1988-43630		19880226
CA 1325497	C	19931221	CA 1988-560029		19880226
AU 8812502	A	19880901	AU 1988-12502		19880229
AU 612626	B2	19910718			
PRIORITY APPLN. INFO.:			JP 1987-46454	A	19870227
			JP 1987-115144	A	19870512
			JP 1987-206146	A	19870818
			JP 1987-289017	A	19871116

OTHER SOURCE(S): CASREACT 110:154893; MARPAT 110:154893

GI



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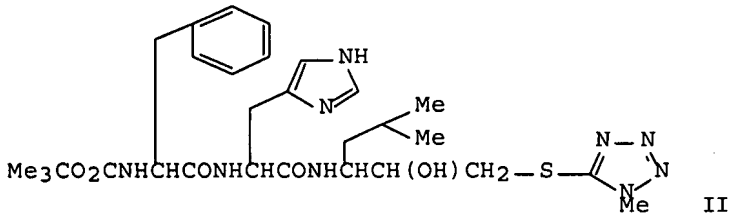


II

AB The title compds. [I; R1 = alkoxycarbonyl, alkoxycarbonylamino, (substituted) alkyl, etc.; R2 = Ph, naphthyl; R3 = C1-6 alkyl, cyclohexyl, Ph; R4 = O2NCH2, alkoxycarbonyl, CH2S(O)nR6; R5 = H, C1-6 alkyl; R6 = (substituted) heterocyclyl; n = 0-2] useful as renin inhibitors, were prepared BOC-Phe-His-NHNH2 in DMF at -10° was treated with HCl/dioxane/isoamyl nitrite; the mixture was stirred 30 min at -30° and N-methylmorpholine was added. 3-Amino-5-methyl-1-(1-methyl-5- tetrazolylthio)-2-hexanol in DMF was added and the mixture was kept overnight in a cold room to give peptide derivative II. I inhibited human plasma renin with IC50 values of 5 + 10-10 to 4 + 10-9 M.

IT ***119832-39-2P***

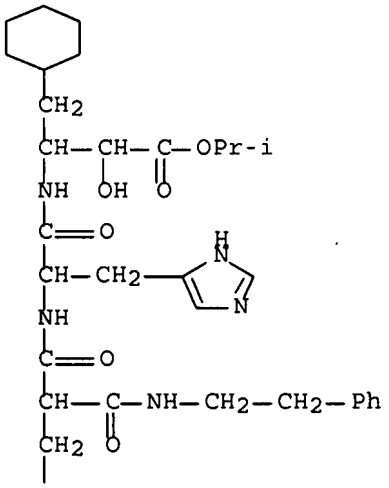
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of, as renin inhibitor)

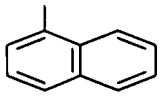
RN 119832-39-2 CAPLUS

CN L-Histidinamide, 2-(1-naphthalenylmethyl)-3-oxo-N-(2-phenylethyl)-β-alanyl-N-[1-(cyclohexylmethyl)-2-hydroxy-3-(1-methylethoxy)-3-oxopropyl]-(9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

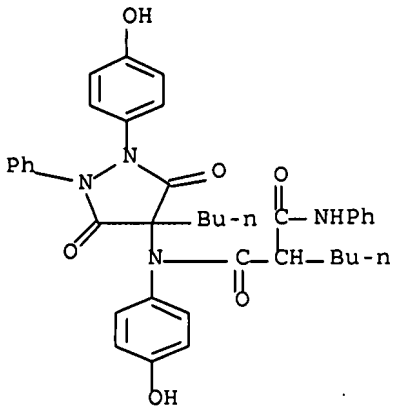


L53 ANSWER 39 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:412218 CAPLUS Full-text
DOCUMENT NUMBER: 105:12218
TITLE: Stability-indicating assay for oxyphenbutazone. Part II. High-performance liquid chromatographic determination of oxyphenbutazone and its degradation products
AUTHOR(S): Fabre, Huguette; Ramiaramana, Andrianandrasana; Blanchin, Marie Dominique; Mandrou, Bernadette
CORPORATE SOURCE: Lab. Chim. Anal., Fac. Pharm., Montpellier, 34060, Fr.
SOURCE: Analyst (Cambridge, United Kingdom) (1986), 111(2), 133-7
CODEN: ANALAO; ISSN: 0003-2654
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An HPLC method is proposed for the simultaneous determination of oxyphenbutazone (I) [129-20-4] and 6 potential decomposition products, using a reversed-phase column and UV detection. The method is more sensitive than thin-layer chromatog. and allows the determination of 0.1% of each degradation product (with respect to I). It was applied to the anal. of com. tablets, capsules, and ointments.

IT *102712-77-6*
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in presence of oxyphenbutazone, in pharmaceuticals by HPLC)
RN 102712-77-6 CAPLUS

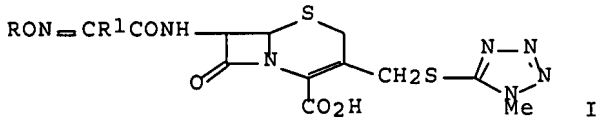
CN Propanediamide, 2-butyl-N-[4-butyl-1-(4-hydroxyphenyl)-3,5-dioxo-2-phenyl-4-pyrazolidinyl]-N-(4-hydroxyphenyl)-N'-phenyl- (9CI) (CA INDEX NAME)



L53 ANSWER 40 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:510633 CAPLUS Full-text
DOCUMENT NUMBER: 101:110633
TITLE: Cephalosporins
INVENTOR(S): Engel Masoliver, Carlos; Inchaurrondo Lasagaboster, Fermin
PATENT ASSIGNEE(S): Laboratorios Fher S. A., Spain
SOURCE: Span., 13 pp.
CODEN: SPXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Spanish
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ES 518223	A1	19840116	ES 1982-518223	19821215

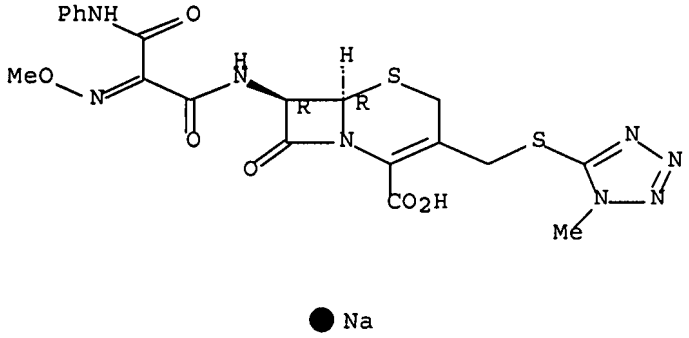
PRIORITY APPLN. INFO.: ES 1982-518223 19821215
GI



AB Cephalosporins I (R = alkyl; R1 = cyano, carbamoyl, alkoxycarbonyl) were prepared Thus, MeO2CCH2CONPh was converted to MeO2CC(:NOH)CONHPh which was methylated and hydrolyzed to give HO2CC(:NOMe)CONHPh (II). I (R = Me, R1 = CONPh) was obtained by acylating the aminocephem with II.
IT ***91530-42-6P 91530-43-7P 91530-47-1P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

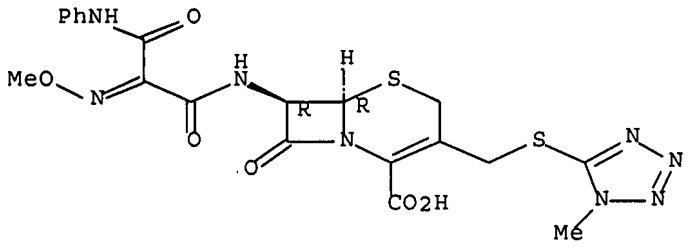
RN 91530-42-6 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[2-(methoxyimino)-1,3-dioxo-3-(phenylamino)propyl]amino]-3-[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-8-oxo-, monosodium salt, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



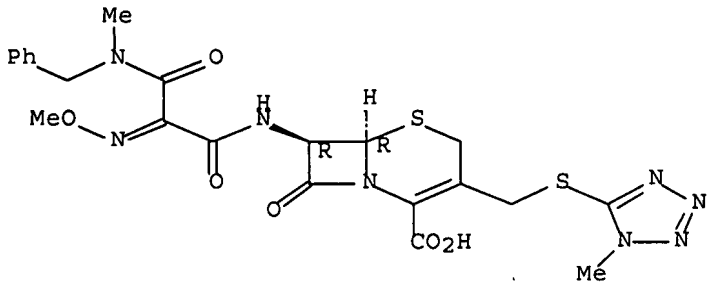
RN 91530-43-7 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[2-(methoxyimino)-1,3-dioxo-3-(phenylamino)propyl]amino]-3-[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



RN 91530-47-1 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[2-(methoxyimino)-3-[methyl(phenylmethyl)amino]-1,3-dioxopropyl]amino]-3-[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L53 ANSWER 41 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:34336 CAPLUS Full-text
DOCUMENT NUMBER: 100:34336
TITLE: Cephalosporin ethers
INVENTOR(S): Scartazzini, Riccardo; Bickel, Hans
PATENT ASSIGNEE(S): Ciba-Geigy Corp. , USA
SOURCE: U.S., 41 pp. Cont.-in-part of U.S. Ser. No. 373,818, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

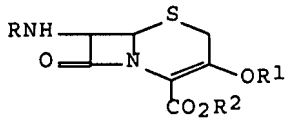
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4405778	A	19830920	US 1976-657904	19760213
CH 587268	A5	19770429	CH 1972-9788	19720629
CH 603666	A5	19780831	CH 1977-1154	19720629
CH 605987	A5	19781013	CH 1972-18722	19721222
CH 605988	A5	19781013	CH 1973-2655	19730223
ZA 7304050	A	19740529	ZA 1973-4050	19730614
SU 542474	A3	19770105	SU 1973-1940203	19730627
SU 677662	A3	19790730	SU 1973-1943362	19730627
AT 7305696	A	19750815	AT 1973-5696	19730628
AT 329745	B	19760525		
ES 416411	A1	19760516	ES 1973-416411	19730628
ES 416412	A1	19760516	ES 1973-416412	19730628
ES 416413	A1	19761116	ES 1973-416413	19730628
HU 172459	B	19780928	HU 1973-CI1599	19730628
PL 93779	B1	19770630	PL 1973-163718	19730629
PL 104396	B1	19790831	PL 1973-173571	19730629
PL 116789	B1	19810630	PL 1973-163715	19730629
NO 7500055	A	19740103	NO 1975-55	19750108
ES 442262	A1	19770701	ES 1975-442262	19751031
CH 597241	A5	19780331	CH 1976-5624	19760505
FI 7902808	A	19790910	FI 1979-2808	19790910
FI 64941	B	19831031		
FI 64941	C	19840210		

PRIORITY APPLN. INFO.:		
CH 1972-9788	A	19720629
CH 1972-12195	A	19720817
CH 1972-18722	A	19721222
CH 1973-2655	A	19730223
US 1973-373818	A2	19730626
CH 1972-2655	A	19730223

CH 1973-7388	A	19730523
FI 1973-1751	A	19730530
NO 1973-2683	A	19730628
CH 1976-5624	A	19760505

OTHER SOURCE(S): MARPAT 100:34336

GI



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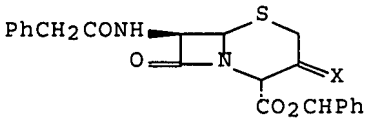


III

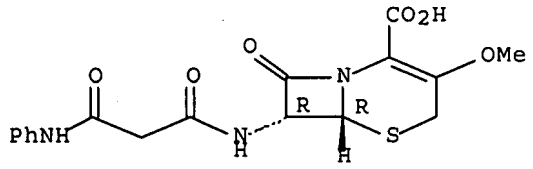
AB Cephalosporins I (R = acyl; R1 = alkyl; R2 = ester group) were prepared Thus, I (R = PhCH2CO, R1 = Me, R2 = CHPh2) (II) was prepared by ozonolysis of III (X = CH2) and methylation of the resulting mixture of III (X = O) and its 1-oxide. III (X = CH2) was prepared from Na 7- phenylacetamidocephalosporanate by deacetylation, esterification, iodination, and deiodination. II was deacylated, hydrolyzed to the acid, and reacylated to give numerous acyl derivs.

IT ***51803-52-2P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 51803-52-2 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-3-methoxy-8-oxo-, (6R-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 42 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	1983:558866 CAPLUS Full-text
DOCUMENT NUMBER:	99:158866
TITLE:	Amino acid derivatives and their therapeutic use
INVENTOR(S):	Roques, Bernard; Schwart, Jean Charles; Lecomte, Jeanne Marie
PATENT ASSIGNEE(S):	Fr.
SOURCE:	Eur. Pat. Appl., 105 pp. CODEN: EPXXDW
DOCUMENT TYPE:	Patent
LANGUAGE:	French
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 82088	A1	19830622	EP 1982-402314	19821216
EP 82088	B1	19860402		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
FR 2518088	A1	19830617	FR 1981-23488	19811216
FR 2518088	B1	19871127		
JP 58150547	A	19830907	JP 1982-221060	19821216
JP 03046463	B	19910716		
AT 18902	T	19860415	AT 1982-402314	19821216
US 4618708	A	19861021	US 1985-715764	19850325
US 4738803	A	19880419	US 1986-900814	19860822
PRIORITY APPLN. INFO.:			FR 1981-23488 A	19811216
			US 1982-449687 A1	19821214
			EP 1982-402314 A	19821216
			US 1985-715764 A3	19850325

OTHER SOURCE(S): CASREACT 99:158866; MARPAT 99:158866

AB R-X-Y-Z-CHR1COR2 [R = phosphono, sulfo, amino, carbamoyl, alkyl; X = CH(CH2)nR3 (n = 0-2; R3 = H, (un)substituted alkyl, Ph, naphthyl, cyclohexyl, thienyl, etc.), C:CHR3; Y = CO, NH, CH2CO; Z = CO, NR4 (R4 = alkyl, R1R4 = a ring); R1 = H or (un)substituted alkyl or Ph; R2 = OH or (un)substituted alkyl, phenoxy, amino, etc.] were prepared (101 compds. claimed). Thus, reaction of PhCH2CHBrCO2H with PhCH2ONH2, followed by formylation and coupling with glycine benzyl ester tosylate gave PhCH2ON(CHO)CH(CH2Ph)CO-Gly-OCH2Ph. The products are useful as enkephalinase inhibitors, analgesics, antidepressants, antidiuretics, and hypotensives. Thus, HON(CHO)CH2CH(CH2Ph)CO-Gly-NHCH2C6H4F-p was an effective analgesic, countering the effects of phenylbenzoquinone at 1 mg/kg i.v.

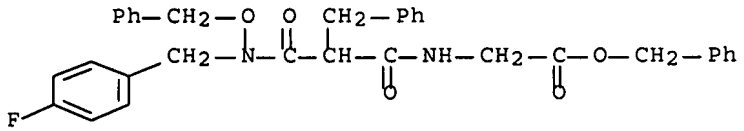
IT ***87438-32-2P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrogenolysis of)

RN 87438-32-2 CAPLUS

CN Glycine, N-[N-[(4-fluorophenyl)methyl]-3-oxo-N-(phenylmethoxy)-2-(phenylmethyl)-β-alanyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



L53 ANSWER 43 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1982:562688 CAPLUS Full-text

DOCUMENT NUMBER: 97:162688

TITLE: Cephalosporins

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

JP 57080390	A	19820519	JP 1980-155394	19801105
PRIORITY APPLN. INFO.:			JP 1980-155394	19801105
OTHER SOURCE(S):	CASREACT 97:162688			

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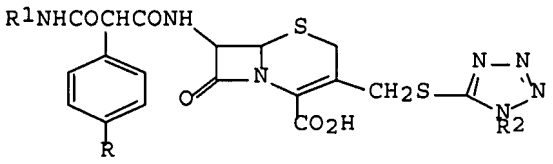

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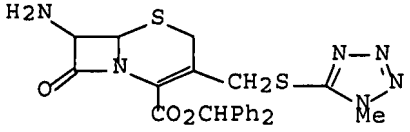
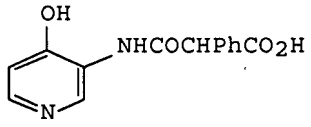


II



III

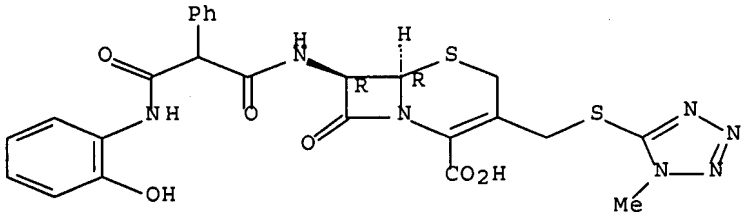
AB Antibiotics I [R = H, OH; R1 = (substituted) Ph, pyridyl, pyrimidyl, quinolinyl; R2 = alkyl] were prepared by, e.g., acylation of II. Thus, stirring 136 mg III with 250 mg II in DMF containing dicyclohexylcarbodiimide at room temperature for 1 h gave 193 mg I (R = H, R1 = 4-hydroxy-3-pyridyl, R2 = Me) benzhydryl ester, which on hydrolysis gave 136 mg I (R = H, R1 = 4-hydroxy-3-pyridyl, R2 = Me). Min. inhibition concns. are given for I against Escherichia coli, Proteus mirabilis, Serratia marcescens and Staphylococcus aureus.

IT ***83255-30-5P 83255-37-2P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antibacterial activity of)

RN 83255-30-5 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[3-[(2-hydroxyphenyl)amino]-1,3-dioxo-2-phenylpropyl]amino]-3-[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-8-oxo-, [6R-(6α,7β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

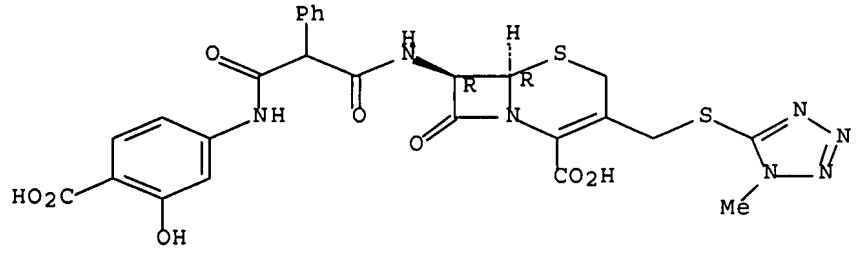


RN 83255-37-2 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[3-[(4-carboxy-3-hydroxyphenyl)amino]-1,3-dioxo-2-phenylpropyl]amino]-3-[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-8-oxo-, [6R-(6α,7β)]-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

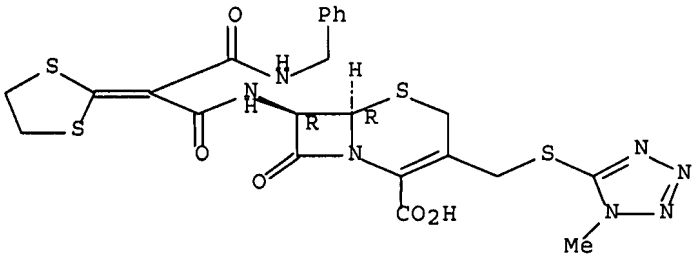


L53 ANSWER 44 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:402717 CAPLUS Full-text
DOCUMENT NUMBER: 97:2717
TITLE: Potent cephalosporinase inhibitors: 7β-[2-(1,3-dithiolan-2-ylidene)acetamido]cephalosporins and related compounds
AUTHOR(S): Ohya, Satoshi; Miyadera, Tetsuo; Yamazaki, Mitsuo
CORPORATE SOURCE: Biol. Res. Lab., Sankyo Co., Ltd., Tokyo, 140, Japan
SOURCE: Antimicrobial Agents and Chemotherapy (1982), 21(4), 613-17
CODEN: AMACCQ; ISSN: 0066-4804
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Cephalosporins possessing a 1,3-dithiolane, 1,3-dithiane, or 1,3-dithietane ring on their 7β-substituents showed potent inhibitory activity against cephaloridine hydrolysis by cephalosporinases purified from Proteus morganii, P. rettgeri, and P. inconstans, which were not inhibited by clavulanic acid, a well-known β-lactamase inhibitor. The mode of inhibition was competitive. The dithiolane cephalosporins themselves were stable against hydrolysis by the β-lactamases tested. A combination of a dithiolane cephalosporin and cephaloridine synergistically inhibited in vitro growth of strains of P. morganii, P. rettgeri, P. inconstans, Enterobacter aerogenes, E. cloacae, and Serratia marcescens.

IT ***81948-88-1***
RL: BIOL (Biological study)
(cephalosporinase inhibition by)
RN 81948-88-1 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[2-(1,3-dithiolan-2-ylidene)-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-3-[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

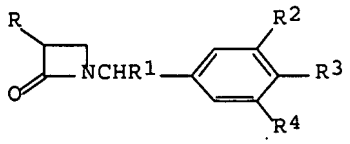
Absolute stereochemistry.



L53 ANSWER 45 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:65461 CAPLUS Full-text
DOCUMENT NUMBER: 94:65461
TITLE: 4-Unsubstituted azetidinone derivatives
INVENTOR(S): Hashimoto, Masashi; Hemmi, Keiji; Kamiya, Takashi; Komori, Tadaaki; Nakaguti, Osamu; Saito, Yoshihisa; Shiokawa, Youichi; Takasugi, Hisahi; Takaya, Takao; Teraji, Tsutomu
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: U.S., 130 pp. Cont.-in-part of U.S. Ser. No. 694,891, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4207234	A	19800610	US 1977-858375	19771207
US 4472300	A	19840918	US 1980-130205	19800313

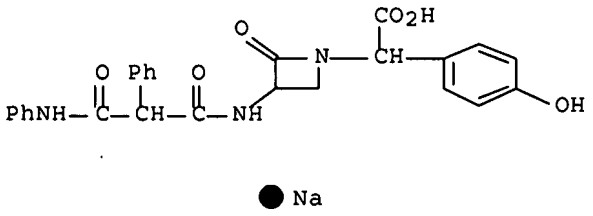
PRIORITY APPLN. INFO.: US 1975-593668 A2 19750707
US 1976-694891 A2 19760610
US 1977-858375 A3 19771207
OTHER SOURCE(S): CASREACT 94:65461; MARPAT 94:65461
GI



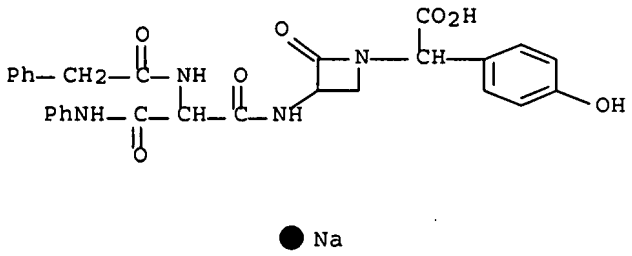
I

AB Lactacillanic acids and analogs I (R = NH2, acylamino, benzenesulfonamido; R1 = CO2H, pharmaceutically acceptable salt or ester derivative of CO2H; R2 = H, NH2, NO2, halo, alkoxy, alkylthio; R3 = H, OH, alkyl, alkylthio, OCH2Ph; R4 = H, Halo, alkoxy, alkylthio), which showed bactericidal activity, were prepared Thus, 3-aminolactacillanic acid reacted with PhCH2COCl in water-Me2CO containing NaHCO3 to yield I (R = PhCH2CONH, R1 = CO2H, R3 = OH, R2 = R4 = H).
IT *59510-12-2P 59510-40-6P*
RL: SPN (Synthetic preparation); PREP (Preparation)

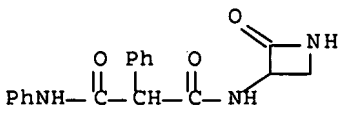
(preparation of)
RN 59510-12-2 CAPLUS
CN 1-Azetidineacetic acid, 3-[[1,3-dioxo-2-phenyl-3-(phenylamino)propyl]amino]-α-(4-hydroxyphenyl)-2-oxo-, monosodium salt (9CI) (CA INDEX NAME)



RN 59510-40-6 CAPLUS
CN 1-Azetidineacetic acid, 3-[[1,3-dioxo-2-[(phenylacetyl)amino]-3-(phenylamino)propyl]amino]-α-(4-hydroxyphenyl)-2-oxo-, monosodium salt (9CI) (CA INDEX NAME)



IT *75263-61-5*
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-alkylation of)
RN 75263-61-5 CAPLUS
CN Propanediamide, N-(2-oxo-3-azetidinyl)-N',2-diphenyl- (9CI) (CA INDEX NAME)



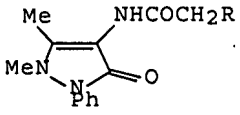
L53 ANSWER 46 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1979:405150 CAPLUS Full-text
DOCUMENT NUMBER: 91:5150
TITLE: Synthesis of 4-(N-substituted-carbamoylacetamido)phenazones, 4-(substituted-

hydrazidocarbonylacetamido)phenazones and N1-(4-phenazonylcarbamoylacetyl)-N2-aroylhydrazines

AUTHOR(S): Abou-Ouf, A. A.; Farghaly, A. M.; El-Kerdawy, M. M.; Massoud, A.
CORPORATE SOURCE: Fac. Pharm., Univ. Mansoura, Mansoura, Egypt

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1978), 16B(11), 989-91
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English

GI

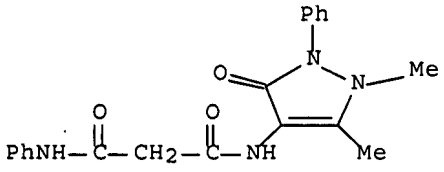


I

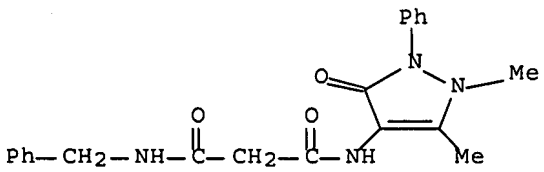
AB 4-Malonamidophenazone Et ester I (R = CO2Et) (II), prepared by the hydrolysis of 4-(2-cyanoacetamido)phenazone I (R = CN) followed by esterification, underwent condensation with R1NH2 (R1 = H, Me, Et, Pr, Ph, PhCH2 4-EtOC6H4) gave I (R = CONHR1,). The hydrazide I (R = CONHNH2) (III), prepared by the reaction of H2HNH2 on II, reacts with R2COR3 (R2 = H, Me; R3 = Ph, substituted Ph) to give I (R = CONHN:CR2R3). The reaction of III with R4Cl (R4 = Bz, PhSO2, etc.) in pyridine or C6H6-Et3N gives the corresponding aroylhydrazines I (R = CONHNHR4). Preliminary pharmacol. screening shows promising results.

IT ***70373-56-7P 70373-57-8P 70373-58-9P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

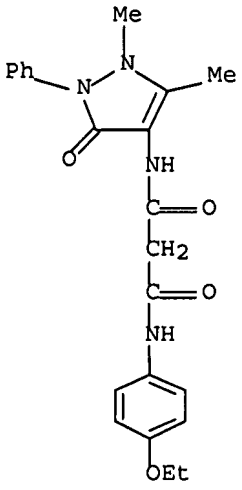
RN 70373-56-7 CAPLUS
CN Propanediamide, N-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-N'-phenyl- (9CI) (CA INDEX NAME)



RN 70373-57-8 CAPLUS
CN Propanediamide, N-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)



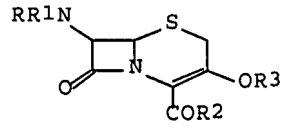
RN 70373-58-9 CAPLUS
CN Propanediamide, N-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-N'-(4-ethoxyphenyl)- (9CI) (CA INDEX NAME)



L53 ANSWER 47 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1979:152207 CAPLUS Full-text
DOCUMENT NUMBER: 90:152207
TITLE: Enol ethers of 7-β-aminocephem-3-ol-4-carboxylic acid derivatives
INVENTOR(S): Scartazzini, Riccardo; Bickel, Hans
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Patentschrift (Switz.), 31 pp. Addn. to Swiss 587,268.
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
CH 605989	A5	19781013	CH 1973-7387		19730523
PRIORITY APPLN. INFO.:			CH 1973-7387	A	19730523

GI



I

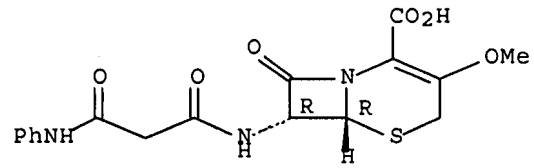
AB The title ethers I [R = NH2-protecting group; R1 = H, acyl; RR1 = bivalent protective group; R2 = CO2H-protecting group; R3 = (substituted) hydrocarbon group] and their 1-oxides and salts were prepared by the reaction of I (R3 = H) or the corresponding ketone with an ester of R3OH with H2SO4, halosulfonic acid or haloalkanesulfonic acid. Thus, I (R = Me3CO2CCHPhCO, R1 = R3 = H, R2 = OCHPh2) reacted with F3CSO3Me in CH2Cl2 to give I (R-R2 = same, R3 = Me).

IT ***51803-52-2P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 51803-52-2 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-3-methoxy-8-oxo-, (6R-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 48 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1978:500769 CAPLUS Full-text

DOCUMENT NUMBER: 89:100769

TITLE: Synthesis for preparation of α-carboxyl and α-carboxy-amido penicillanic and cephalosporanic acid derivatives

AUTHOR(S): Huhn, Magda; Dvortsak, Peter; Zalantai, Livia

CORPORATE SOURCE: Chinoin Chem. and Pharm. Works Ltd., Budapest, Hung.

SOURCE: Curr. Chemother., Proc. Int. Congr. Chemother., 10th (1978), Meeting Date 1977, Volume 1, 569-72. Editor(s): Siegenthaler, Walter; Luethy, Ruedi. Am. Soc. Microbiol.: Washington, D. C.
CODEN: 37XLA2

DOCUMENT TYPE: Conference

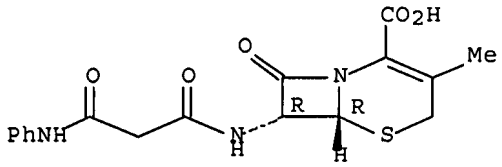
LANGUAGE: English

AB A series of the title derivs. was prepared and tested in vitro for antimicrobial activity. Most derivs. acylated with malonic acids and with hemianilides of phenylmalonic acid showed remarkable activity against Mycobacterium tuberculosis, and gram.-pos. and -neg. microorganisms. In vivo, however, none of the test compds. significantly prolonged the survival time of mice infected i.v. with mycobacteria, even after administration of s.c. doses of 200 mg/kg over 10 days.

IT ***60657-76-3 67371-57-7 67371-58-8***

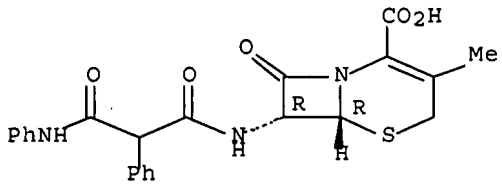
67371-59-9 67371-60-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tuberculostatic activity of)
RN 60657-76-3 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-3-methyl-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



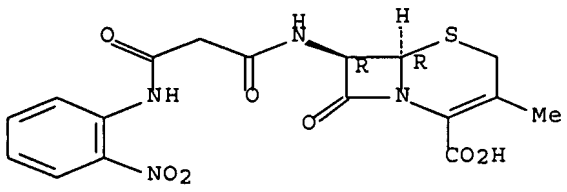
RN 67371-57-7 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[1,3-dioxo-2-phenyl-3-(phenylamino)propyl]amino]-3-methyl-8-oxo-, [6R-(6α,7β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 67371-58-8 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-methyl-7-[[3-[(2-nitrophenyl)amino]-1,3-dioxopropyl]amino]-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

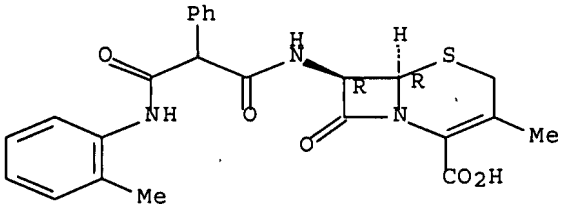
Absolute stereochemistry.



RN 67371-59-9 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

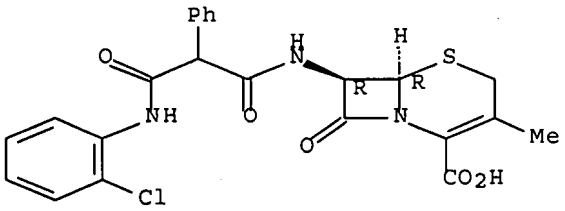
3-methyl-7-[[3-[(2-methylphenyl)amino]-1,3-dioxo-2-phenylpropyl]amino]-8-oxo-, [6R-(6α,7β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

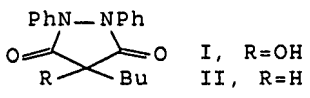


RN 67371-60-2 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[3-[(2-chlorophenyl)amino]-1,3-dioxo-2-phenylpropyl]amino]-3-methyl-8-oxo-, [6R-(6α,7β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 49 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:27732 CAPLUS Full-text
DOCUMENT NUMBER: 88:27732
TITLE: 4-Hydroxyphenylbutazone: a potentially immunogenic contaminant of phenylbutazone preparations
AUTHOR(S): Bundgaard, Hans
CORPORATE SOURCE: Dep. Pharm., R. Dan. Sch. Pharm., Copenhagen, Den.
SOURCE: Archiv for Pharmaci og Chemi, Scientific Edition (1977), 5(4), 87-96
CODEN: AVPCCS; ISSN: 0302-248X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



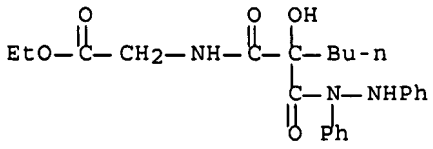
I, R=OH
II, R=H

AB 4-Hydroxyphenylbutazone (I) [16860-43-8], a commonly occurring contaminant in clin. used phenylbutazone (II) [50-33-9] prepns., reacted readily with amines (RNH2) (in aqueous solns., at physiol. pH and temperature) in contrast to the parent drug, with the formation of amides n-butyltartronic acid mono(N,N'-diphenyl)hydrazide amides [PhNHNPhCOC(Bu)(OH)CONHR]. An irreversible reaction occurred with serum albumin at alkaline pH. Comparison of the rate consts. for aminolysis of I under similar conditions showed that this compound was .apprx.25-fold more reactive with glycylglycine [556-50-3] than was benzylpenicillin. This suggested I is a potential immunogenic contaminant, possibly involved in clin. allergic reactions to I prepns.

IT ***64725-03-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 64725-03-7 CAPLUS

CN Hexanoic acid, 2-[[(2-ethoxy-2-oxoethyl)amino]carbonyl]-2-hydroxy-, 1,2-diphenylhydrazide (9CI) (CA INDEX NAME)



L53 ANSWER 50 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:606428 CAPLUS Full-text

DOCUMENT NUMBER: 87:206428

TITLE: 4-Hydroxyphenylbutazone: a potentially immunogenic contaminant of phenylbutazone preparations

AUTHOR(S): Bundgaard, Hans

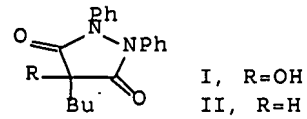
CORPORATE SOURCE: Dep. Pharm., R. Dan. Sch. Pharm., Copenhagen, Den.

SOURCE: Archiv for Pharmaci og Chemi, Scientific Edition (1977), 5(4), 901-10
Published in: Arch. Pharm. Chemi 84(18)
CODEN: AVPCCS; ISSN: 0302-248X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I, R=OH
II, R=H

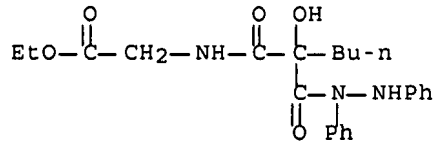
AB A chemical reactivity study of a commonly occurring contaminant, 4-hydroxyphenylbutazone (I) [16860-43-8], in clin. used phenylbutazone (II) [50-33-9] prepns. indicated that in contrast to II, I reacted readily with amines (RNH2) in aqueous solns. at physiol. pH and temperature, with formation n-

butyltartronic acid mono-N,N'-diphenylhydrazide amides [RNHCOC(Bu)(OH)CONPhNHPh]. An irreversible reaction with serum albumin took place at alkaline pH. The contaminant reacted .apprx.25-fold more readily with glycylglycine [556-50-3] than benzylpenicillin and was potentially an immunogenic substance, possibly involved in clin. allergic reactions to I prepns.

IT *64725-03-7*
RL: BIOL (Biological study)
(as hydroxyphenylbutazone aminolysis product, in phenylbutazone pharmaceuticals)

RN 64725-03-7 CAPLUS

CN Hexanoic acid, 2-[[(2-ethoxy-2-oxoethyl)amino]carbonyl]-2-hydroxy-, 1,2-diphenylhydrazide (9CI) (CA INDEX NAME)



L53 ANSWER 51 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:535287 CAPLUS Full-text

DOCUMENT NUMBER: 87:135287

TITLE: Acylation of 6-aminopenicillanic acid, 7-aminocephalosporanic acid, and 7-aminodeacetoxycephalosporanic acid and their derivatives

INVENTOR(S): Diago Meseguer, Jose; Fernandez Lizarbe, Jose Ramon; Palomo Coll, Antonio Luis; Zugaza Bilbao, Alvaro

PATENT ASSIGNEE(S): Gema S. A., Spain; Antibioticos S. A.

SOURCE: Ger. Offen., 31 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

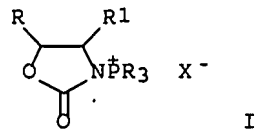
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2701751	A1	19770721	DE 1977-2701751	19770118
ES 444470	A1	19770516	ES 1976-444470	19760120
NL 7700570	A	19770722	NL 1977-570	19770120

PRIORITY APPLN. INFO.: ES 1976-444470 A 19760120

GI



I

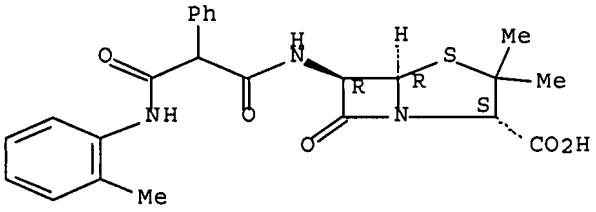
AB The title acids were acylated with 2,5-(O2N)2C6H4CO2H, thienylacetic acid, PhCHClCO2H, N3CHPhCO2H, etc; by preparing a salt of the acylating acid with an organic base, e.g., Et3N, which was treated with I (R = Cl, Br, Me2N, R = R1 = H, Me; X = Br, Cl) to give a mixture of active species with varying content of acid chloride, N-acyl-2-oxazolidinone, and 2-acyloxy-Δ2- oxazoline. The title acids were then added to this mixture to give the N-acyl derivative

IT ***34093-30-6P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 34093-30-6 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-6-[[3-[(2-methylphenyl)amino]-1,3-dioxo-2-phenylpropyl]amino]-7-oxo-, [2S-(2α,5α,6β)]- (9CI) (CA INDEX NAME)

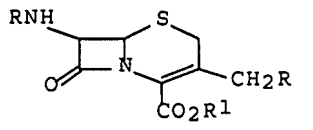
Absolute stereochemistry.



L53 ANSWER 52 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:543125 CAPLUS Full-text
DOCUMENT NUMBER: 85:143125
TITLE: Cephalosporins
INVENTOR(S): Shibuya, Chisei; Ito, Hirataka; Usubuchi, Yutaka; Yamawaki, Naokuni; Ichikawa, Yasushi
PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 51054578	A	19760513	JP 1974-127562	19741107

PRIORITY APPLN. INFO.: JP 1974-127562 A 19741107
GI



I, R=R2R3NCOCH2CO
II, R=H

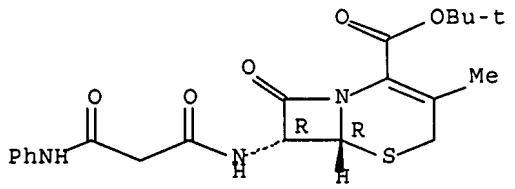
AB Cephalosporins I (R = H, OH, alkanoyloxy, quaternary ammonium, thiadiazolylthio, tetrazolylthio, etc.; R1 = H, alkyl, aralkyl, trisubstituted silyl, phenacyl, alkanoyloxymethyl, salt-forming ion, etc., or RR11 form a lactam ring; R2 and R3 = H, alkyl, aryl, aralkyl, heterocyclyl, alkoxycarbonyl, etc., or R2R3 = alkylene, alkenylene, but not R2 = H and R3 = aliphatic hydrocarbon group) were prepared by acylating II with acids R2R3NCOCH2CO2H or their reactive derivs. I are antibacterial agents (no data). Thus, 0.93 g PhNHCOCH2CO2H was treated with ClCO2Et and then with 1.33 g II (R = H, R1 = CMe3) and Et3N in CHCl3 to give 2.12 g I (R = R2 = H, R1 = CMe3, R3 = Ph). Deprotection with CF3CO2H gave I (R = R1 = R2 = H, R3 = Ph). Also prepared was I (R = OAc, R1 = H, R2 = Me, R3 = Ph).

IT ***60657-75-2P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)

RN 60657-75-2 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-3-methyl-8-oxo-, 1,1-dimethylethyl ester, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

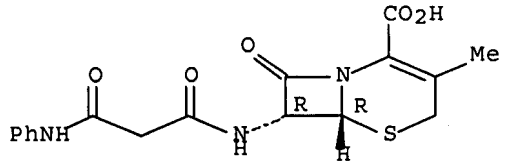


IT ***60657-76-3P 60657-77-4P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 60657-76-3 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-3-methyl-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

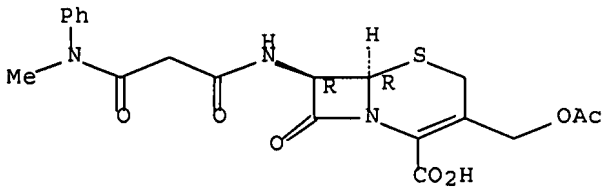
Absolute stereochemistry.



RN 60657-77-4 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[3-(methylphenylamino)-1,3-dioxopropyl]amino]-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



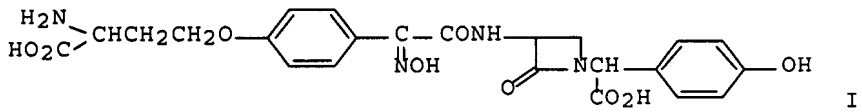
L53 ANSWER 53 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:421078 CAPLUS Full-text
DOCUMENT NUMBER: 85:21078
TITLE: Azetidinone derivatives
INVENTOR(S): Kamiya, Takashi; Yoshihisa, Takarazuka; Hashimoto, Masashi; Teraji, Tsutomu; Takaya, Takao; Komori, Tadaaki; Nakaguti, Osamu; Oku, Teruo; Shiokawa, Youichi; et al.
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: Ger. Offen., 318 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2529941	A1	19760408	DE 1975-2529941	19750704
JP 51125061	A	19761101	JP 1974-77091	19740704
JP 51125062	A	19761101	JP 1974-85526	19740724
JP 51125064	A	19761101	JP 1974-88452	19740731
JP 51075056	A	19760629	JP 1975-2650	19741223
BE 830934	A1	19760102	BE 1975-157924	19750702
CH 618161	A5	19800715	CH 1975-8634	19750702
DK 7503023	A	19760105	DK 1975-3023	19750703
FI 7501949	A	19760105	FI 1975-1949	19750703
NO 7502419	A	19760106	NO 1975-2419	19750703
FR 2278335	A1	19760213	FR 1975-20990	19750703
FR 2278335	B1	19821217		
SE 428799	B	19830725	SE 1975-7683	19750703
SE 428799	C	19831103		
NL 7508008	A	19760106	NL 1975-8008	19750704
AU 7582778	A	19770106	AU 1975-82778	19750704
ES 439134	A1	19770301	ES 1975-439134	19750704
ZA 7504306	A	19770525	ZA 1975-4306	19750704
GB 1519495	A	19780726	GB 1975-28394	19750704
HU 172476	B	19780928	HU 1975-FU336	19750704
AT 7505170	A	19790715	AT 1975-5170	19750704
AT 355034	B	19800211		
CA 1063108	A1	19790925	CA 1975-230828	19750704
AT 7806099	A	19790915	AT 1978-6099	19780822
AT 7806098	A	19800415	AT 1978-6098	19780822
AT 359514	B	19801110		
SE 7903460	A	19790419	SE 1979-3460	19790419
SE 7903504	A	19790420	SE 1979-3504	19790420
CH 637924	A5	19830831	CH 1980-5357	19800711

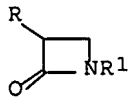
PRIORITY APPLN. INFO.:

JP 1974-77091	A	19740704
JP 1974-85526	A	19740724
JP 1974-88452	A	19740731
JP 1975-2650	A	19741223
JP 1974-100159	A	19740830
JP 1974-101712	A	19740902
JP 1974-102288	A	19740904
JP 1974-136561	A	19741126
JP 1974-138137	A	19741129
JP 1975-3779	A	19741225
JP 1975-1272	A	19741228
JP 1975-16584	A	19750207
JP 1975-18241	A	19750212
JP 1974-30356	A	19750312
JP 1975-30356	A	19750312
JP 1975-32702	A	19750317
JP 1975-32703	A	19750317
JP 1975-33292	A	19750318
JP 1975-34830	A	19750319
JP 1975-33821	A	19750320
JP 1975-33822	A	19750320
CH 1975-8634	A	19750702
AT 1975-5170	A	19750704

GI



I



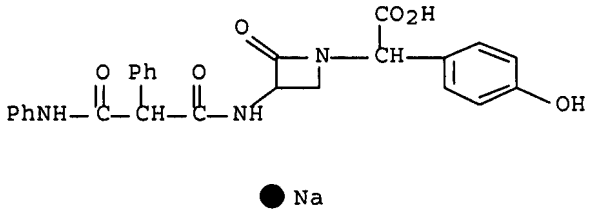
II

AB After the antibiotic FR-1923 (obtained from fermentation liquor of Nocardia) was identified as I, 543 analogs [II; R = NH2 or acylamino; R1 = alkyl (saturated or unsatd., straight-chain or branched) with substituents, e.g., CO2H (or its derivs.), CN, OH, NH2, Ph or substituted Ph] were prepared by standard procedures and shown to be effective against, e.g., Bacillus subtilis, Escherichia coli, and Staphylococcus aureus.

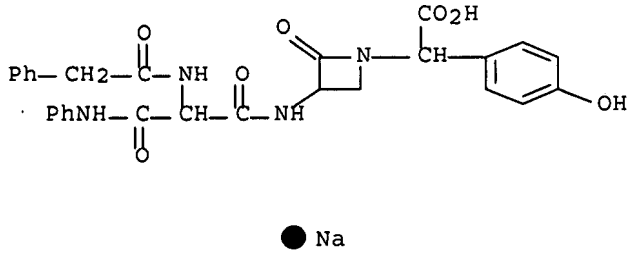
IT ***59510-12-2P 59510-40-6P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 59510-12-2 CAPLUS

CN 1-Azetidineacetic acid, 3-[[1,3-dioxo-2-phenyl-3-(phenylamino)propyl]amino]-α-(4-hydroxyphenyl)-2-oxo-, monosodium salt (9CI) (CA INDEX NAME)



RN 59510-40-6 CAPLUS
CN 1-Azetidineacetic acid, 3-[[1,3-dioxo-2-[(phenylacetyl)amino]-3-(phenylamino)propyl]amino]-α-(4-hydroxyphenyl)-2-oxo-, monosodium salt (9CI) (CA INDEX NAME)



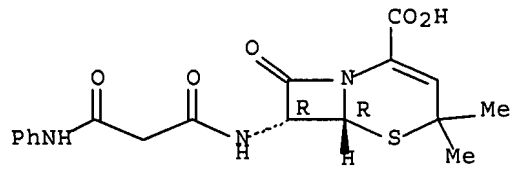
L53 ANSWER 54 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1975:514441 CAPLUS Full-text
DOCUMENT NUMBER: 83:114441
TITLE: 7-(N-Acylamino)-2,2-dimethyl-3-cephem-4-carboxylic acids and their esters
INVENTOR(S): Heusler, Karl; Bickel, Hans; Fechtig, Bruno; Peter, Heinrich; Scartazzini, Riccardo
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Patentschrift (Switz.), 25 pp.
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 562250	A5	19750530	CH 1970-8472	19700605
ES 391895	A1	19730701	ES 1971-391895	19710603
NL 7107730	A	19711207	NL 1971-7730	19710604
PRIORITY APPLN. INFO.:			CH 1970-8472 A	19700605

GI For diagram(s), see printed CA Issue.
AB Cephems I (R = H2NCHPh, MeO2CCH2, EtO2CCH2, BrCH2, PhNHCOCH2, MeOCH2, 4-aminopyridiniummethyl, PhOCH2, 4-MeC6H4SCH2, AcCH2, BzCH2, NCCH2, NCCHMe, NCCHPh, ClCH2CH2NH, ClCH2CH2, ClCH2, Cl2CH, allyl, PhCH2, 2-thienylmethyl, MeSCH2, (MeO2C)2CH, HO2CCHPh, amino(2-thienyl)methyl, 1-tetrazolylmethyl, 1-methyl-2-imidazolylmethyl, 1,2,4-triazol-3- ylthiomethyl, BF2CH, N3CH2) were prepared by acylating the 7-aminocephem, prepared from penicillins G or V in 15 steps.

IT *35621-40-0P*
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35621-40-0 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-4,4-dimethyl-8-oxo-,
(6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

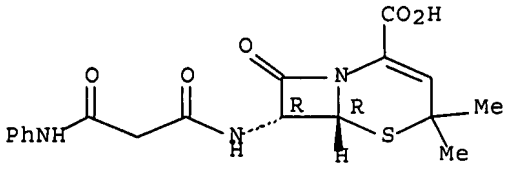


L53 ANSWER 55 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:437556 CAPLUS Full-text
DOCUMENT NUMBER: 81:37556
TITLE: 7-Amino-2,2-dimethylceph-3-em-4-carboxylic acid derivatives
INVENTOR(S): Heusler, Karl; Bickel, Hans; Fechtig, Bruno; Peter, Heinrich; Scartazzini, Riccardo
PATENT ASSIGNEE(S): Ciba-Geigy A.-G.
SOURCE: Brit., 50 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
GB 1353326	A	19740515	GB 1971-5052		19710219
PRIORITY APPLN. INFO.:			GB 1971-5052	A	19710219

GI For diagram(s), see printed CA Issue.
AB Thirty-four title compds. I (R = H, acyl; R1 = H, Me, CMe3, CH2COC6H4Br-p, Na), useful as bactericides were prepared Me2SO oxidation of the azetidinones II (R = PhCH2-CO, PhOCH2CO; R1 = CMe3), prepared from penicillin G and V, resp., gave the corresponding title compds. I which on hydrolysis and deacylation gave I (R = R1 = H). Most I (R = acyl) were prepared by acylation of I (R = R1 = H).
IT *35621-40-0P*
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35621-40-0 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-4,4-dimethyl-8-oxo-,
(6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 56 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:108513 CAPLUS Full-text
DOCUMENT NUMBER: 80:108513
TITLE: Isoxazolyl derivatives of penicillin and cephalosporin
PATENT ASSIGNEE(S): Koninklijke Nederlandsche Gist- en Spiritusfabriek N. V.
SOURCE: Ger. Offen., 73 pp. Division of Ger. Offen. 2,155,081 (CA 77;48483b).
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2166468	A1	19740214	DE 1971-2166468	19711105
US 3891635	A	19750624	US 1971-195482	19711103
BE 775012	A1	19720505	BE 1971-110230	19711105
NL 7115231	A	19720509	NL 1971-15231	19711105
FR 2112504	A5	19720616	FR 1971-39822	19711105
FR 2112504	B1	19751031		
ZA 7107433	A	19720726	ZA 1971-7433	19711105
HU 162822	B	19730428	HU 1971-KO2471	19711105
AU 7135431	A	19730510	AU 1971-35431	19711105
ES 396720	A1	19750416	ES 1971-396720	19711105
CA 983920	A1	19760217	CA 1971-126985	19711105
CH 572935	A5	19760227	CH 1975-14002	19711105
CH 572936	A5	19760227	CH 1975-14003	19711105
CH 573436	A5	19760315	CH 1971-16162	19711105
SU 520050	A3	19760630	SU 1971-1713952	19711105
JP 52012200	B	19770405	JP 1971-88177	19711105
CA 993442	A2	19760720	CA 1973-166365	19730319
ES 423795	A1	19761216	ES 1974-423795	19740301
US 4010264	A	19770301	US 1974-533708	19741217

PRIORITY APPLN. INFO.: GB 1970-53040 A 19701106
US 1971-195482 A2 19711103
CA 1971-126985 A3 19711105

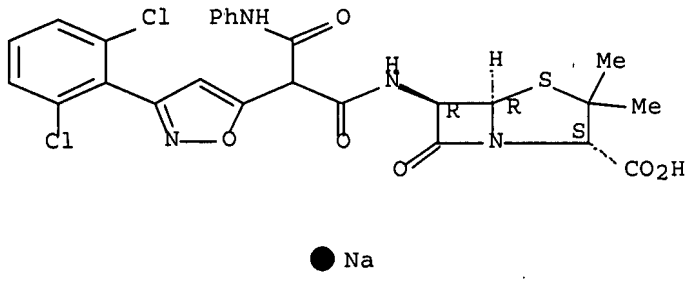
GI For diagram(s), see printed CA Issue.

AB Penicillins I (R = 2,6-Cl2C6H3, 2,4,6-Me3C6H2, 4-O2NC6H4, 1-adamantanyl, Me; R1 = H, Me, CO2H, CONH2, CN; R2 = H, Cl, Me, NHCO2CH2C6H4NO2-p, NH2, CONH2, CONHPh) and their salts were prepared by converting 6-aminopenicillanic acid to its trimethylsilyl ester followed by treatment with the isoxazolylacetyl chloride or by treating trimethylsilyl 6-isocyanatopenicillanate with the isoxazolylacetic acid. The cephalosporins II (R = 2,6-Cl2C6H3, 2,4,6-Me3C6H2, 4-O2NC6H4, Me; R1 = H, Me; R3 = H, OAc) were similarly prepared

IT ***36923-10-1P***
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 36923-10-1 CAPLUS
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[2-[3-(2,6-dichlorophenyl)-5-isoxazolyl]-1,3-dioxo-3-(phenylamino)propyl]amino]-3,3-dimethyl-7-oxo-, monosodium salt, [2S-(2α,5α,6β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 57 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:108511 CAPLUS Full-text
DOCUMENT NUMBER: 80:108511
TITLE: Penicillin and cephalosporin derivatives
PATENT ASSIGNEE(S): Koninklijke Nederlandsche Gist- en Spiritusfabriek N. V.
SOURCE: Ger. Offen., 75 pp. Division of Ger. Offen. 2,155,081 (CA 77;48483b).
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2166467	A1	19740214	DE 1971-2166467	19711105
US 3891635	A	19750624	US 1971-195482	19711103
BE 775012	A1	19720505	BE 1971-110230	19711105
NL 7115231	A	19720509	NL 1971-15231	19711105
FR 2112504	A5	19720616	FR 1971-39822	19711105
FR 2112504	B1	19751031		
ZA 7107433	A	19720726	ZA 1971-7433	19711105
HU 162822	B	19730428	HU 1971-KO2471	19711105
AU 7135431	A	19730510	AU 1971-35431	19711105
ES 396720	A1	19750416	ES 1971-396720	19711105
CA 983920	A1	19760217	CA 1971-126985	19711105
CH 572935	A5	19760227	CH 1975-14002	19711105
CH 572936	A5	19760227	CH 1975-14003	19711105
CH 573436	A5	19760315	CH 1971-16162	19711105
SU 520050	A3	19760630	SU 1971-1713952	19711105
JP 52012200	B	19770405	JP 1971-88177	19711105
CA 993442	A2	19760720	CA 1973-166365	19730319
ES 423795	A1	19761216	ES 1974-423795	19740301
US 4010264	A	19770301	US 1974-533708	19741217
PRIORITY APPLN. INFO.:			GB 1970-53040 A	19701106

US 1971-195482 A2 19711103
CA 1971-126985 A3 19711105

GI For diagram(s), see printed CA Issue.

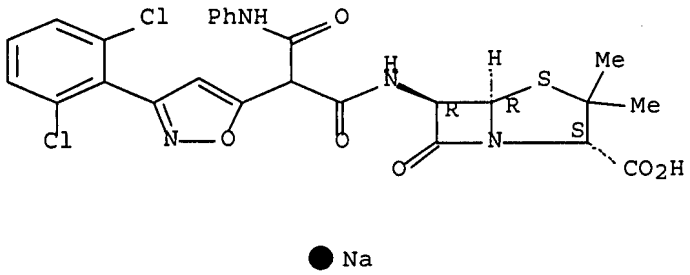
AB Penicillins I (R = 2,6-Cl2C6H3, 2,4,6-Me3C6H2, 4-O2NC6H4, 1-adamantanyl, Me; R1 = H, Me, CO2H, CONH2, CN; R2 = H, Cl, Me, NHCO2CH2C6H4NO2-p, NH2, CONH2, CONHPh) and their salts were prepared by converting 6-amino-penicillanic acid to its trimethylsilyl ester followed by treatment with the isoxazolylacetyl chloride or by treating trimethylsilyl 6-isocyanatopenicillanate with the isoxazolylacetic acid. The cephalosporins II (R = 2,6-Cl2C6H3, 2,4,6-Me3C6H2, 4-O2NC6H4, Me; R1 = H, Me; R3 = H, OAc) were similarly prepared

IT ***36923-10-1P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 36923-10-1 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[2-[3-(2,6-dichlorophenyl)-5-isoxazolyl]-1,3-dioxo-3-(phenylamino)propyl]amino]-3,3-dimethyl-7-oxo-, monosodium salt, [2S-(2α,5α,6β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 58 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:83019 CAPLUS Full-text
DOCUMENT NUMBER: 80:83019
TITLE: Enol derivatives
INVENTOR(S): Scartazzini, Riccardo; Bickel, Hans
PATENT ASSIGNEE(S): Ciba-Geigy A.-G.
SOURCE: Ger. Offen., 263 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2331133	A1	19740117	DE 1973-2331133	19730619
DE 2331133	C2	19840412		
CH 587268	A5	19770429	CH 1972-9788	19720629
CH 603666	A5	19780831	CH 1977-1154	19720629
CH 605987	A5	19781013	CH 1972-18722	19721222
CH 605988	A5	19781013	CH 1973-2655	19730223
FI 59601	B	19810529	FI 1973-1750	19730530
FI 59601	C	19810910		
FI 59602	B	19810529	FI 1973-1751	19730530

FI 59602	C	19810910		
FI 60870	B	19811231	FI 1973-1752	19730530
FI 60870	C	19820413		
SE 417099	B	19810223	SE 1973-8234	19730612
SE 417099	C	19810611		
SE 417429	B	19810316	SE 1973-8233	19730612
SE 417429	C	19810702		
SE 417430	B	19810316	SE 1973-8235	19730612
SE 417430	C	19810702		
ZA 7304050	A	19740529	ZA 1973-4050	19730614
RO 63761	A1	19781215	RO 1973-860064	19730614
RO 64419	A2	19790310	RO 1973-86374	19730614
RO 64226	A1	19790515	RO 1973-75138	19730614
RO 73345	A1	19820909	RO 1973-84759	19730614
FR 2190418	A1	19740201	FR 1973-23235	19730626
AU 7357386	A	19750109	AU 1973-57386	19730627
GB 1435111	A	19760512	GB 1973-30537	19730627
SU 542474	A3	19770105	SU 1973-1940203	19730627
SU 677662	A3	19790730	SU 1973-1943362	19730627
BE 801597	A1	19731228	BE 1973-132845	19730628
DD 106184	A5	19740612	DD 1973-171903	19730628
DD 106187	A5	19740612	DD 1973-171906	19730628
DD 107470	A5	19740812	DD 1973-171905	19730628
AT 7305694	A	19750415	AT 1973-5694	19730628
AT 356809	B	19800527		
AT 7305695	A	19750615	AT 1973-5695	19730628
AT 356810	B	19800527		
AT 7305696	A	19750815	AT 1973-5696	19730628
AT 329745	B	19760525		
AT 7500576	A	19750815	AT 1975-576	19730628
AT 329762	B	19760525		
HU 167726	B	19751225	HU 1973-CI1393	19730628
HU 168017	B	19760228	HU 1973-CI1392	19730628
ES 416411	A1	19760516	ES 1973-416411	19730628
ES 416412	A1	19760516	ES 1973-416412	19730628
HU 169032	B	19760928	HU 1973-CI1391	19730628
ES 416413	A1	19761116	ES 1973-416413	19730628
HU 172459	B	19780928	HU 1973-CI1599	19730628
CA 1110230	A1	19811006	CA 1973-175100	19730628
NO 145240	B	19811102	NO 1973-2681	19730628
NO 145240	C	19820210		
NO 145241	B	19811102	NO 1973-2682	19730628
NO 145241	C	19820210		
NO 145242	B	19811102	NO 1973-2683	19730628
NO 145242	C	19820210		
DK 153324	B	19880704	DK 1973-3588	19730628
NL 7309136	A	19740102	NL 1973-9136	19730629
NL 7309137	A	19740102	NL 1973-9137	19730629
NL 7309139	A	19740102	NL 1973-9139	19730629
JP 49049986	A	19740515	JP 1973-74353	19730629
JP 59034716	B	19840824		
JP 49049987	A	19740515	JP 1973-74354	19730629
JP 59033598	B	19840816		
JP 49049988	A	19740515	JP 1973-74355	19730629
JP 59033599	B	19840816		
PL 91608	B1	19770331	PL 1973-163719	19730629
PL 93779	B1	19770630	PL 1973-163718	19730629
PL 104396	B1	19790831	PL 1973-173571	19730629
PL 116789	B1	19810630	PL 1973-163715	19730629
NO 7500055	A	19740103	NO 1975-55	19750108

ES 442262	A1	19770701	ES 1975-442262	19751031
CH 597241	A5	19780331	CH 1976-5624	19760505
SE 7612053	A	19761029	SE 1976-12053	19761029
SE 435289	B	19840917		
SE 435289	C	19841220		
FI 7902808	A	19790910	FI 1979-2808	19790910
FI 64941	B	19831031		
FI 64941	C	19840210		
JP 55105690	A	19800813	JP 1979-169493	19791227
JP 59034196	B	19840821		
JP 55105691	A	19800813	JP 1979-169494	19791227
JP 59051957	B	19841217		
JP 55105692	A	19800813	JP 1979-169495	19791227
JP 59038955	B	19840920		
JP 56039093	A	19810414	JP 1980-94119	19800711
JP 60019916	B	19850518		
JP 56049390	A	19810502	JP 1980-99283	19800718
JP 61008071	B	19860311		
JP 56068684	A	19810609	JP 1980-99282	19800718
JP 61008070	B	19860311		
JP 56127392	A	19811006	JP 1981-17382	19810207
JP 59007716	B	19840220		
JP 59076089	A	19840428	JP 1983-146770	19830812
JP 60054320	B	19851129		
JP 59076090	A	19840428	JP 1983-146771	19830812
JP 60053037	B	19851122		

PRIORITY APPLN. INFO.:	CH 1972-9788	A	19720629
	CH 1972-12195	A	19720817
	CH 1972-18722	A	19721222
	CH 1973-2655	A	19730223
	CH 1972-2655	A	19730223
	CH 1973-7388	A	19730523
	FI 1973-1751	A	19730530
	NO 1973-2683	A	19730628
	CH 1976-5624	A	19760505

GI For diagram(s), see printed CA Issue.

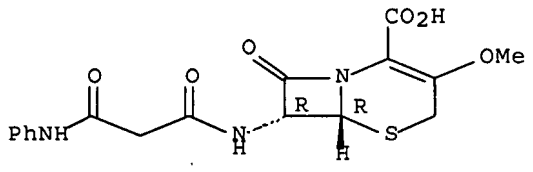
AB 7-Acylamino-3-alkoxycephemcarboxylic acids I (R = acyl, R1 = OMe, OEt, OBu, OCH2Ph, OAc) were prepared Thus, the Na salt of I (R = PhCH2CO, R1 = CH2OH) was converted to its diphenylmethyl ester, iodinated, and dehydroiodinated to the cepham II (X = CH2), which on ozonolysis gave a mixture of II (X = O) and its 1-oxide. Treatment of the mixture with CH2N2 gave I (R = PhCH2CO, R1 = OMe), its 1-oxide, and its 2-cephem analog, which was separated by chromatog.

IT ***51803-52-2P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 51803-52-2 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-3-methoxy-8-oxo-, (6R-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

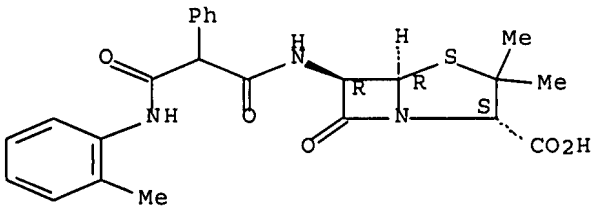


L53 ANSWER 59 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:82957 CAPLUS Full-text
DOCUMENT NUMBER: 80:82957
TITLE: Semisynthetic penicillins
INVENTOR(S): Palomo Coll, Antonio L.
PATENT ASSIGNEE(S): gema S. A.
SOURCE: Span., 9 pp. Addn. to Span. 376,271 (See Ger. 2,105,166 (CA 75;151782f).
CODEN: SPXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Spanish
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ES 386962	A2	19730401	ES 1970-386962	19701231
BE 762311	A1	19710701	BE 1971-99209	19710129
CH 549049	A	19740515	CH 1971-1624	19710202
DE 2105166	A	19710902	DE 1971-2105166	19710204
NL 7101575	A	19710809	NL 1971-1575	19710205
AT 314730	B	19740425	AT 1971-972	19710205
PRIORITY APPLN. INFO.:			ES 1970-376271 A	19700205
			ES 1970-386962 A	19701231

GI For diagram(s), see printed CA Issue.
AB The penicillin I (R = 0-MeC6H4NHCO) was prepared by treating 6-aminopenicillanic acid (II) with 0-MeC6H4NHCOCHPhCO2H in the presence of Me2N+:-CHCl-.ClSO2H. I (R = NHCONHN:CMe2) was prepared by treating II with Me2C:NNHCONHCHPhCO2H. I (R = NHCONHN:CHPh) was similarly prepared
IT ***34093-30-6P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 34093-30-6 CAPLUS
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-6-[[3-[(2-methylphenyl)amino]-1,3-dioxo-2-phenylpropyl]amino]-7-oxo-, [2S-(2α,5α,6β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 60 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:514397 CAPLUS Full-text
DOCUMENT NUMBER: 77:114397
TITLE: 8-Oxo-5-thia-1-azabicyclo[4,2,0]oct-2-ene compounds

INVENTOR(S): Heusler, Karl; Bickel, Hans; Fechtig, Bruno; Peter, Heinrich; Scartazzini, Riccardo
PATENT ASSIGNEE(S): Ciba-Geigy A. G.
SOURCE: S. African, 130 pp.
CODEN: SFXXAB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ZA 7102523		19711125	ZA 1971-2523	19710420

GI For diagram(s), see printed CA Issue.

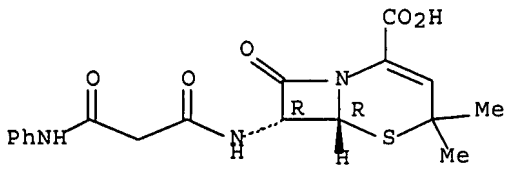
AB Tert-Bu α-[4β-[2-(hydroxymethyl)-2-propylthio]-2-oxo-3β-(N- phenylacetamido)-1-azetidinyl]-α-(triphenylphosphoranylidene)- acetate (I) was treated with Ac2O in Me2SO to give the ceph(3)-em-4-carboxylic acid (II, R = PhCH2CO, R1 = tert-Bu). Penicillin G azide was heated to give 2,2-dimethyl-6-(N-phenylacetamido)-3-[(2,2,2- trichloroethoxycarbonyl)amino]penam (III). III was treated with HOAc and the product treated with NaBH4 to give 4β-[2-(hydroxymethyl)-2- propylthio]-3β-(N-phenylacetamido)azetidinon-2-one, which was converted to I. About 40 II (R = PhOCH2CO, H, PhCHNH2CO, MeO2CCH2CO, BrCH2CO, PhNHCOCH2CO, NCCH2CO, H2C:CHCH2CO, 2-thienylacetyl, MeSCH2CO, 2-imidazolylthioacetyl etc.; R1 = tert-Bu, H, p-BrC6H4COCH2) were prepared

IT ***35621-40-0P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35621-40-0 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-4,4-dimethyl-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 61 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:448483 CAPLUS Full-text
DOCUMENT NUMBER: 77:48483
TITLE: (Isoxazolylacetamido)penicillanic and -cephalosporanic acid derivatives
PATENT ASSIGNEE(S): Koninklijke Nederlandsche Gist- en Spiritusfabriek N. V.
SOURCE: Ger. Offen., 79 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2155081	A	19720510	DE 1971-2155081	19711105
DE 2155081	B2	19750515		
DE 2155081	C3	19751218		
US 3891635	A	19750624	US 1971-195482	19711103
BE 775012	A1	19720505	BE 1971-110230	19711105
NL 7115231	A	19720509	NL 1971-15231	19711105
FR 2112504	A5	19720616	FR 1971-39822	19711105
FR 2112504	B1	19751031		
ZA 7107433	A	19720726	ZA 1971-7433	19711105
HU 162822	B	19730428	HU 1971-KO2471	19711105
AU 7135431	A	19730510	AU 1971-35431	19711105
ES 396720	A1	19750416	ES 1971-396720	19711105
CA 983920	A1	19760217	CA 1971-126985	19711105
CH 572935	A5	19760227	CH 1975-14002	19711105
CH 572936	A5	19760227	CH 1975-14003	19711105
CH 573436	A5	19760315	CH 1971-16162	19711105
SU 520050	A3	19760630	SU 1971-1713952	19711105
JP 52012200	B	19770405	JP 1971-88177	19711105
CA 993442	A2	19760720	CA 1973-166365	19730319
ES 423795	A1	19761216	ES 1974-423795	19740301
US 4010264	A	19770301	US 1974-533708	19741217
PRIORITY APPLN. INFO.:			GB 1970-53040 A	19701106
			US 1971-195482 A2	19711103
			CA 1971-126985 A3	19711105

GI For diagram(s), see printed CA Issue.

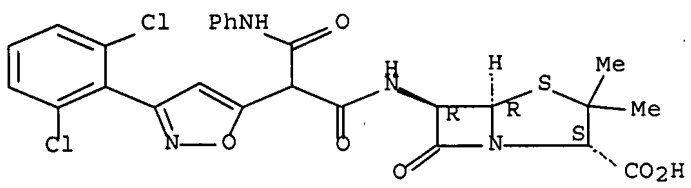
AB Twenty-three title compds. (I; Q = Q1 or Q2; R = 2,6-Cl2C6H3, 2,4,6-Me3C6H2, 1-adamantyl, p-O2NC6H4, or Me; R1 = H, CO2H, Me, CONH2, or CN; R2 = H, Cl, Me, p-O2NC6H4CH2O2CNH, NH2, H2NCO, or PhNHCO; R3 = H or OAc) or their Na or cyclohexylamine salts, useful as antibiotics, were prepared by amidation of the acetyl chlorides II (X = Cl). Thus, Et3N and Me3SiCl were added to Q1NH2 in AcOEt under N at .apprx.0°, the mixture was kept 35 min, II (R = 2,6-Cl2C6H3, R1 = R2 = H) in AcOEt added at <5°, and the mixture kept 90 min at room temperature to give 32% I (Q = Q1 = R = 2,6-Cl2C6H3, R1 = R2 = H) as Na salt (III). III was also obtained by reaction of II (X = OH) with Q1NCO (Me3Si ester) in the presence of N-vinylimidazole catalyst.

IT ***36923-10-1P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 36923-10-1 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[2-[3-(2,6-dichlorophenyl)-5-isoxazolyl]-1,3-dioxo-3-(phenylamino)propyl]amino]-3,3-dimethyl-7-oxo-, monosodium salt, [2S-(2α,5α,6β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Na

L53 ANSWER 62 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:99686 CAPLUS Full-text
DOCUMENT NUMBER: 76:99686
TITLE: Pharmacologically active 8-oxo-5-thia-1-azabicyclo[4,2,0]oct-2-ene
INVENTOR(S): Heusler, Karl; Bickel, Hans; Fechtig, Bruno; Peter, Heinrich; Scartazzini, Riccardo
PATENT ASSIGNEE(S): Ciba-Geigy A.-G.
SOURCE: Ger. Offen., 175 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2127287	A	19711216	DE 1971-2127287	19710602
CH 563396	A5	19750630	CH 1970-8470	19700605
US 3883517	A	19750513	US 1971-149341	19710602
ES 391893	A1	19740616	ES 1971-391893	19710603
NL 7107726	A	19711207	NL 1971-7726	19710604
BE 768173	A1	19711207	BE 1971-104318	19710607
FR 2097836	A5	19720303	FR 1971-20461	19710607
FR 2100727	A1	19720324	FR 1971-20459	19710607
FR 2100727	A5	19720324		

PRIORITY APPLN. INFO.:
CH 1970-8470 A 19700605
CH 1971-242 A 19710108
CH 1971-7279 A 19710517

GI For diagram(s), see printed CA Issue.

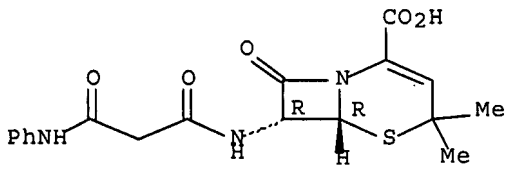
AB The cephalosporin derivs. I (R = PhCH2, PhOCH2, Me3CO2CNHCHPh, AcCH2, EtO2CCH2, BrCH2, PhNHCOCH2, MeOCH2, PhOCH2, p-Me-C6H4SCH2, BzCH2, NCCH2, NCCHMe, NCCHPr, ClCH2CH2NH, ClCH2CH2, ClCH2, Cl2CH, allyl, 2-thienylmethyl, MeSCH2, (MeO2C)2CH, HO2CCHPh, amino(2-thienyl)methyl, 1-tetrazolylmethyl, BrCH2, Br2CH, N3CH2, (1-methyl-2- imidazolyl)thiomethyl, 1,2,4-triazol-3-ylthiomethyl) and some esters and internal salts were prepared by cyclizing the azetidinones II (R1 = PhCH2CO, PhOCH2CO), hydrolyzing to II (R1 = H), and treating this with RCO2H, RCO2Na, or RCOCl. I did not undergo isomerization of the double bond owing to the 2 Me groups in the 2-position. They are active against penicillin-resistant Staphylococcus aureus.

IT ***35621-40-0P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35621-40-0 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-4,4-dimethyl-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 63 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:551782 CAPLUS Full-text
DOCUMENT NUMBER: 75:151782
TITLE: α-(Carbamoyl)benzylpenicillins
INVENTOR(S): Palomo Coll, Antonio L.
PATENT ASSIGNEE(S): Gema S.A.
SOURCE: Ger. Offen., 24 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 2105166	A	19710902	DE 1971-2105166		19710204
ES 376271	A1	19720316	ES 1970-376271		19700205
ES 386962	A2	19730401	ES 1970-386962		19701231
PRIORITY APPLN. INFO.:			ES 1970-376271	A	19700205
			ES 1970-386962	A	19701231

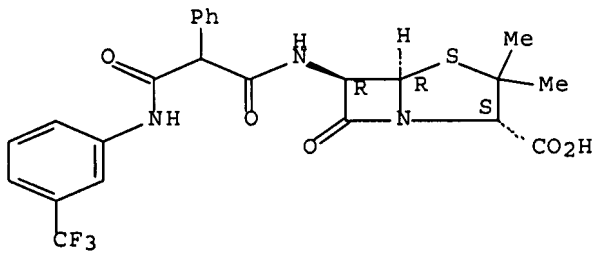
GI For diagram(s), see printed CA Issue.

AB The title compds. [I; R=Et, o-MeC6H4, m-F3CC6H4; R1=H or Et; NRR1=morpholino] were prepared by reaction of 6-aminopenicillanic acid (II) with RNR1COCHPhCO2H and ClSO2CH:N+NH2 Cl- (III). Thus, III was added to HO2CCHPhCONHC6H4Me-o in CH2Cl2 at -5°, stirred 1 hr at 10°, added to II in CH2Cl2-Et3N-pivalic acid, and stirred with aqueous HCHO solution to give 90% I (R=o-MeC6H4, R1=H). Similarly prepared were 3 other I.

IT ***34093-28-2P 34093-30-6P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

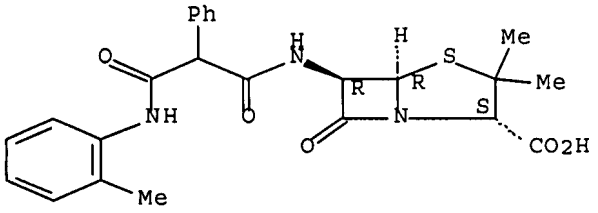
RN 34093-28-2 CAPLUS
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-7-oxo-6-[2-phenyl-2-[(α,α,α-trifluoro-m-tolyl)carbamoyl]acetamido]- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 34093-30-6 CAPLUS
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-6-[[3-[(2-methylphenyl)amino]-1,3-dioxo-2-phenylpropyl]amino]-7-oxo-, [2S-(2α,5α,6β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 64 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:59552 CAPLUS
DOCUMENT NUMBER: 55:59552
ORIGINAL REFERENCE NO.: 55:11438b-e
TITLE: Derivatives of dichloromalonic acid
INVENTOR(S): Heymons, Albrecht; Liebig, Horst
PATENT ASSIGNEE(S): Riedel de Haen Akt.-Ges.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

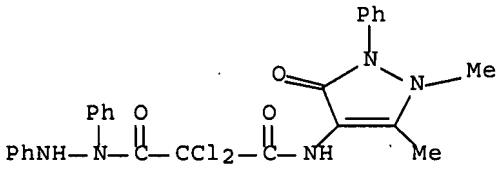
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1075628		19600218	DE	

AB Mono- and dihydrazides and cyclic monohydrazides of dichloromalonic acid, with antidiabetic action on peroral administration, were prepared by dichlorination of 3,5-dioxopyrazolidines and cleaving the product to the desired derivative by adding alcs., amines, or alkanolamines. 1,2-Diphenyl-3,5-dioxopyrazolidine (I) heated in CHCl3 5 hrs. at 70° with Cl passed in gave 70% 1,2-diphenyl-4,4-dichloro-3,5- dioxopyrazolidine (II), m. 112-15°. I (0.1 mole) with 0.11 mole AlCl3 in 150 cc. CHCl3 then Cl gave 75% II. II (1.6 g.) with 1.7 g. NaOAc and 4 cc. MeOH gave 97% dichloromalonic acid Me ester 1,2- diphenylhydrazide, m. 159°. II (3 g.) with 1 cc. pyridine and 30 cc. iso-PrOH gave 60% dichloromalonic acid iso-Pr ester 1,2-diphenylhydrazide, m. 153-66° (decomposition). II with Et2NCH2CH2OH in dioxane gave 94% dichloromalonic acid diethylaminoethyl ester 1,2-diphenylhydrazide (III), m. 84-5° (decomposition). III with 0.1N HCl gave 78% dichloromalonic acid 1,2-diphenylhydrazide, m. 144-5°. II with PhNH2 in dioxane gave 72% dichloromalonic acid anilide 1,2-diphenylhydrazide, m. 186-7°. II with 4-amino-1-phenyl-2,3- dimethyl-5-pyrazolone in dioxane gave dichloromalonic acid 1,2-diphenylhydrazide 1-phenyl-2,3-dimethyl-5-pyrazolon-4-ylamide, m. 187-93° (decomposition).

IT ***114398-45-7P***, Malonamic acid, N-antipyrinyl-2,2-dichloro-, 1,2-diphenylhydrazide
RL: PREP (Preparation)
(preparation of)

RN 114398-45-7 CAPLUS
CN Malonamic acid, N-antipyrinyl-2,2-dichloro-, 1,2-diphenylhydrazide (6CI)

(CA INDEX NAME)



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L5              1 SEA ABB=ON  PLU=ON  US2004-767784/AP
                  D SCA
L6              1 SEA ABB=ON  PLU=ON  L4 AND L5
                  D SCA

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                  D SCA L7

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                741672-93-5/BI OR 741672-94-6/BI OR 741672-95-7/BI OR 741672-96
                -8/BI OR 741672-97-9/BI OR 741672-98-0/BI OR 741672-99-1/BI OR
                741673-00-7/BI OR 741673-01-8/BI OR 741673-02-9/BI OR 741673-03
                -0/BI OR 741673-04-1/BI OR 741673-05-2/BI OR 741673-06-3/BI OR
                741673-07-4/BI OR 741673-08-5/BI OR 741673-09-6/BI OR 741673-10
                -9/BI OR 741673-11-0/BI OR 741673-12-1/BI OR 741673-13-2/BI OR
                741673-14-3/BI OR 741673-15-4/BI OR 741673-16-5/BI OR 741673-17
                -6/BI OR 741673-18-7/BI OR 741673-19-8/BI OR 741673-20-1/BI OR
                741673-21-2/BI OR 741673-22-3/BI OR 741673-23-4/BI OR 741673-24
                -5/BI OR 741673-25-6/BI OR 741673-26-7/BI OR 741673-27-8/BI OR
                741673-28-9/BI OR 741673-29-0/BI OR 741673-30-3/BI OR 741673-31
                -4/BI OR 741673-32-5/BI OR 741673-33-6/BI OR 741673-34-7/BI OR
                741673-35-8/BI OR 741673-36-9/BI OR 741673-37-0/BI OR 741673-38
                -1/BI OR 741673-39-2/BI OR 741673-40-5/BI OR 741673-41-6/BI OR
                741673-42-7/BI OR 741673-43-8/BI OR 741673-44-9/BI OR 741673-45
                -0/BI OR 741673-46-1/BI OR 741673-47-2/BI OR 741673-48-3/BI OR
                741673-49-4/BI OR 741673-50-7/BI OR 741673-51-8/BI OR 741673-52
                -9/BI OR 741673-53-0/BI OR 741673-54-1/BI OR 741

     FILE 'CAPLUS' ENTERED AT 13:16:13 ON 02 MAY 2007
L16            1 SEA ABB=ON  PLU=ON  L15

     FILE 'STNGUIDE' ENTERED AT 13:17:13 ON 02 MAY 2007

     FILE 'REGISTRY' ENTERED AT 13:22:27 ON 02 MAY 2007
L17       149780 SEA ABB=ON  PLU=ON  NC2NC3/ESS
L18           27 SEA ABB=ON  PLU=ON  L17 AND L15
                 D SCA
                 E "PROPANEDIAMIDE, N-(5-BENZOYL-2,3,4,5-TETRAHYDRO-1-METHYL-2-O
L19           27 SEA ABB=ON  PLU=ON  L12 AND L17

     FILE 'CAPLUS' ENTERED AT 13:36:08 ON 02 MAY 2007
L20            1 SEA ABB=ON  PLU=ON  L19

     FILE 'REGISTRY' ENTERED AT 13:38:20 ON 02 MAY 2007
L21          197 SEA ABB=ON  PLU=ON  L12 NOT L15

     FILE 'CAPLUS' ENTERED AT 13:38:39 ON 02 MAY 2007
L22           70 SEA ABB=ON  PLU=ON  L21
L23              ANALYZE PLU=ON  L13 1- RN :    5445 TERMS
                 D

     FILE 'REGISTRY' ENTERED AT 13:40:57 ON 02 MAY 2007
L24            1 SEA ABB=ON  PLU=ON  146420-49-7
                 D SCA
L25          369 SEA ABB=ON  PLU=ON  L12 NOT L24

     FILE 'CAPLUS' ENTERED AT 13:41:49 ON 02 MAY 2007
L26           65 SEA ABB=ON  PLU=ON  L25

     FILE 'REGISTRY' ENTERED AT 13:42:08 ON 02 MAY 2007
L27            1 SEA ABB=ON  PLU=ON  13734-34-4
                 D SCA
L28            1 SEA ABB=ON  PLU=ON  143301-52-4
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                D SCA
L29             1 SEA ABB=ON  PLU=ON  147140-68-9
                D SCA
L30           369 SEA ABB=ON  PLU=ON  L25 NOT (L28 OR L29)

     FILE 'CAPLUS' ENTERED AT 13:44:33 ON 02 MAY 2007
L31            65 SEA ABB=ON  PLU=ON  L30

     FILE 'STNGUIDE' ENTERED AT 13:45:14 ON 02 MAY 2007

     FILE 'REGISTRY' ENTERED AT 13:48:54 ON 02 MAY 2007
                D SCA L19
L32             0 SEA ABB=ON  PLU=ON  " PROPANEDIAMIDE, N-(5-BENZOYL-2,3,4,5-TETR
                AHYDRO-1-METHYL-2-OXO-1H-1,5-BENZODIAZEPIN-3-YL)-N'-[(3,5-DIFLU
                OROPHENYL)METHYL)-2-METHYL-"/CN
                E "PROPANEDIAMIDE, N-(5-BENZOYL-2,3,4,5-TETRAHYDRO-1-METHYL-2-O
                E "PROPANEDIAMIDE, N-(5-BENZOYL-2,3,4,5-TETRAHYDRO-1-METHYL-2-O
L33             1 SEA ABB=ON  PLU=ON  "PROPANEDIAMIDE, N-(5-BENZOYL-2,3,4,5-TETRA
                HYDRO-1-METHYL-2-OXO-1H-1,5-BENZODIAZEPIN-3-YL)-N'-((3,5-DIFLUO
                ROPHENYL)METHYL)-2-METHYL-"/CN
                D SCA

     FILE 'REGISTRY' ENTERED AT 13:51:39 ON 02 MAY 2007
                D IDE L33
L34             STRUCTURE UPLOADED

     FILE 'MARPAT' ENTERED AT 13:55:33 ON 02 MAY 2007
L35             9 SEA SSS SAM L9
L36             0 SEA SSS SAM L34
L37             2 SEA SSS FUL L34
L38             1 SEA ABB=ON  PLU=ON  L37/COM

     FILE 'MARPAT' ENTERED AT 13:57:06 ON 02 MAY 2007
                D STAT QUE L38
                D IBIB ABS QHIT L38 1

     FILE 'CAPLUS' ENTERED AT 13:58:13 ON 02 MAY 2007
L39            32 SEA ABB=ON  PLU=ON  GALLEY G?/AU
L40             4 SEA ABB=ON  PLU=ON  GOERGLER A?/AU
L41           297 SEA ABB=ON  PLU=ON  JACOBSEN H?/AU
L42            45 SEA ABB=ON  PLU=ON  KITAS E?/AU
L43          2834 SEA ABB=ON  PLU=ON  PETERS J?/AU
L44             9 SEA ABB=ON  PLU=ON  L39 AND (L40 OR L41 OR L42 OR L43)
L45             1 SEA ABB=ON  PLU=ON  L40 AND (L41 OR L42 OR L43)
L46             1 SEA ABB=ON  PLU=ON  L41 AND (L42 OR L43)
L47             3 SEA ABB=ON  PLU=ON  L42 AND L43
L48             9 SEA ABB=ON  PLU=ON  (L44 OR L45 OR L46 OR L47)
L49             2 SEA ABB=ON  PLU=ON  (L39 OR L40 OR L41 OR L42 OR L43) AND (L8
                OR L26)

     FILE 'REGISTRY' ENTERED AT 14:00:33 ON 02 MAY 2007

     FILE 'CAPLUS' ENTERED AT 14:00:36 ON 02 MAY 2007
                D STAT QUE L16
                D STAT QUE L48
                D STAT QUE L49
L50             9 SEA ABB=ON  PLU=ON  (L16 OR (L48 OR L49))
                D IBIB ABS HITIND L50 1-9

     FILE 'BEILSTEIN' ENTERED AT 14:01:53 ON 02 MAY 2007
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L51             0 SEA SSS SAM L34
L52             0 SEA SSS FUL L34

     FILE 'REGISTRY' ENTERED AT 14:02:35 ON 02 MAY 2007

     FILE 'CAPLUS' ENTERED AT 14:02:38 ON 02 MAY 2007
               D STAT QUE L8
               D STAT QUE L26
L53            64 SEA ABB=ON  PLU=ON  (L8 OR L26) NOT L50
               D IBIB ABS HITSTR L53 1-64


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:    1 MAY 2007  HIGHEST RN 934050-43-8
     DICTIONARY FILE UPDATES:   1 MAY 2007  HIGHEST RN 934050-43-8

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     TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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     REGISTRY includes numerically searchable data for experimental and
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     experimental property data in the original document.  For information
     on property searching in REGISTRY, refer to:

     http://www.cas.org/support/stngen/stndoc/properties.html

     FILE CAPLUS

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     FILE COVERS 1907 - 2 May 2007  VOL 146 ISS 19
     FILE LAST UPDATED: 1 May 2007  (20070501/ED)

     Effective October 17, 2005, revised CAS Information Use Policies apply.
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     http://www.cas.org/infopolicy.html

     FILE STNGUIDE
     FILE CONTAINS CURRENT INFORMATION.
     LAST RELOADED: Apr 27, 2007 (20070427/UP).

     FILE MARPAT
```

FILE CONTENT: 1961-PRESENT VOL 146 ISS 18 (20070427/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 2007060644 15 MAR 2007
DE 102006023116 15 MAR 2007
EP 1762248 14 MAR 2007
JP 2007059877 08 MAR 2007
WO 2007030662 15 MAR 2007
GB 2429975 14 MAR 2007
FR 2890657 16 MAR 2007
RU 2295953 27 MAR 2007
CA 2556850 24 FEB 2007

Expanded G-group definition display now available.

FILE BEILSTEIN
FILE LAST UPDATED ON April 02, 2007

FILE COVERS 1771 TO 2006.
FILE CONTAINS 9,882,697 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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*****************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.           *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE     *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                   *
* FOR PRICE INFORMATION SEE HELP COST                           *
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```

NEW

* ***PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.***
* ***NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.***

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